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Heat Capacity of Liquids: Volume I Critical Review and Recommended Values

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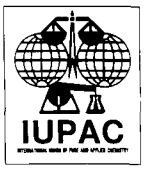

In association with the
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Foreword

The *Journal of Physical and Chemical Reference Data* is published jointly by the American Institute of Physics and the American Chemical Society for the National Institute of Standards and Technology (NIST). Its objective is to provide critically evaluated physical and chemical property data, fully documented as to the original sources and the criteria used for evaluation. One of the principal sources of material for the journal is the NIST Standard Reference Data Program, a program promoting the compilation and critical evaluation of property data.

The regular issues of the *Journal of Physical and Chemical Reference Data* are published bimonthly and contain compilations and critical data reviews of moderate length. Longer works, volumes of collected tables, and other material unsuited to a periodical format have previously been published as *Supplements to the Journal*. Beginning in 1989 the generic title of these works was changed to *Monograph*, which reflects their character as independent publications. This volume, "Heat Capacity of Liquids: Volumes I and II. Critical Review and Recommended Values" by Milan Zábranský, Vlastimil Růžička Jr., Vladimír Majer, and Eugene S. Domalski is the first of two volumes of *Monograph No. 6* of the *Journal of Physical and Chemical Reference Data.*

Jean W. Gallagher, Editor
Journal of Physical and Chemical Reference Data

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The Commission I.2 on Thermodynamics of the International Union of Pure and Applied Chemistry is responsible, through its Subcommittee on Thermodynamic Data, for the dissemination of internationally-approved thermodynamic tables. The projects are conveniently discussed under two headings. Firstly, there is the compilation of internationally-agreed values for the equilibrium thermodynamic properties of individual substances of special interest and importance to scientists and technologists. This work is carried out at the IUPAC Thermodynamic Tables Project Centre at Imperial College of Science, Technology and Medicine, London with publication in the series International Thermodynamic Tables of the Fluid State, now published by Blackwell Scientific Publications, Oxford. The second type of project is the critical compilation of values for individual equilibrium properties for a large group of compounds, which is carried out through international collaboration. The present publication on Heat Capacities of Liquids is the result of the first of these projects to be approved, because of the importance of this property in thermochemistry, in thermodynamics and in chemical engineering generally. The authors are to be congratulated on their careful assessment of all the experimental data and the clear presentation of their results: the summary of the experimental data, the selected and rejected sets, the coefficients in the correlating equations, the recommended data and the deviation plots. The tables given here should be of considerable value to all thermodynamicists. The emphasis on the accuracy of the values will be of particular importance to the user.

J. H. Dymond
Chairman
Subcommittee on Thermodynamic Data
Commission I.2 on Thermodynamics
International Union of Pure and Applied Chemistry

Preface 2

This monograph is a result of an IUPAC data project carried out in cooperation with the Department of Physical Chemistry at the Institute of Chemical Technology, Prague (Czech Republic), the Laboratory of Thermodynamics and Chemical Engineering at the University Blaise Pascal in Clermont-Ferrand (France) and the Chemical Thermodynamics and Kinetics Division at the National Institute of Standards and Technology (NIST), Gaithersburg, MD (U.S.A). The authors started cooperation on data collection and evaluation of liquid heat capacities in the mid-1980s, and this endeavor was accepted as an official project of the IUPAC Subcommittee on Thermodynamic Data (STD) of the Commission on the Chemical Thermodynamics in 1987 at the 34th IUPAC General Assembly in Boston. A specimen copy including all introductory material and representative examples of tables was prepared in the spring of 1991 and sent for review to experts from all over the world selected by STD. Altogether eleven reviews were received, providing constructive criticisms and suggestions. As a collective group, they accepted the project output in a positive manner without any serious objections. Most reports from reviewers were available before the 36th IUPAC General Assembly held in Hamburg in 1991 where all the input from the review process was discussed and minor modifications to the text and data presentation were decided upon. The manuscript was corrected accordingly and final approval for publication was given by the IUPAC Commission on Chemical Thermodynamics in the summer of 1992 during its meeting at Snowbird, Utah. Although STD and the authors were approached by several scientific book publishers, the *Journal of Physical and Chemical Reference Data* Monograph Series was selected as the best possible choice to publish the results of the IUPAC data project. This Monograph Series was selected because the NIST Standard Reference Data Program (SRDP) from which it originates has considerable experience in the dissemination of evaluated data and also because it is in charge of distributing a computerized database on liquid heat capacities which is closely connected with this data project. All the materials for publishing the monograph were submitted electronically to the SRDP staff during 1994.

The objective of the data project was to collect and critically assess all calorimetric, isobaric, and saturation heat capacities for well-defined organic and inorganic compounds in the liquid state which were published in the primary literature between 1862 and 1994. Older data were considered in exceptional cases where no other literature sources were found. Only pure chemicals with melting temperature below 573 K were considered. High melting chemicals such as most metals, inorganic compounds, and some organic compounds, were not included. The collected heat capacity data were related mainly to atmospheric pressure or saturated vapor pressure while investigations which focused on heat capacities as a function of pressure were considered beyond the scope of this project. The main outputs of the project are the recommended heat capacities provided as a function of temperature along the saturation line in the form of correlation equation(s) parameters and tabulated values with the expected uncertainties. Detailed characterization of all literature sources of experimental data (both included and rejected in the final selection) is also given.

The authors have followed, in general, the terminology and symbols recommended by IUPAC as well as the values for fundamental constants and molar masses. With respect to nomenclature, the authors followed the system used by Chemical Abstracts Service because it was generally an unambiguous and computer readable scheme.

At this point, we wish to thank all those who contributed to the success of the project in its different stages.

First of all we are grateful to the successive Chairmen at the Department of Physical Chemistry, Institute of Chemical Technology, Prague — J. Pick, R. Holub and J. Matouš, for allowing us to use Department facilities for most of the practical work of the project. We thank the Chief of the Standard Reference Data Program, M. W. Chase, Jr., and the Editor of the Journal of Physical and Chemical Reference Data, J. W. Gallagher, for their assistance with arrangements in the final publication phase of the project. The Chairman of the Subcommittee on Thermodynamic Data, J. H. Dymond, was always instrumental and ready to help when problems had to be overcome.

Our sincere thanks go to all the reviewers who devoted their valuable time to reading the specimen copy. Their ideas and remarks certainly improved the manuscript and affected the final version of the book in a positive manner. The individual reviewers were: R. C. Chirico from NIPER, Bartlesville, OK (U.S.A.), G. T. Furukawa from NIST, Gaithersburg, MD (U.S.A.), A. I. Johns from the National Engineering Laboratory, Glasgow (United Kingdom), B. V. Lebedev from the Lobachevsky State University, Nizhnii Novgorod (Russia), P. Liley from Purdue University, IN (U.S.A.), K. N. Marsh from The Texas A&M University System, TX (U.S.A.), P. A. G. O'Hare from NIST, Gaithersburg, MD (U.S.A.), H. Suga from the University of Osaka (Japan), I. Wadsö from the University of Lund (Sweden), E. F. Westrum, Jr. from the University of Michigan, Ann Arbor, MI (U.S.A.) and E. Wilhelm from the Vienna University (Austria). Reviews by P. A. G. O'Hare and E. F. Westrum, Jr., were especially detailed and helpful, once again many thanks.

Regarding problems with nomenclature, our valuable advisors were F. Liška and M. Ferles, professors of organic chemistry at the Institute of Chemical Technology, Prague. The program for cubic spline fitting was made available to us through the courtesy of K. Kollár-Hunek from the Budapest Technical University. Deviation plots were generated by using a library of Fortran subroutines known as VolksGrapher which were kindly provided to us by W. E. Anderson from NIST, Gaithersburg, MD. All figures for the monograph were carefully prepared by J. Margoliusová from the Institute of Chemical Technology in Prague. We also want to acknowledge help in the literature search given to us by all librarians in the Central Library (directed at the time by K. Sgallová) at the Institute of Chemical Technology, Prague as well as help from many unnamed staff persons in more than ten scientific libraries in the Czech Republic and abroad. Last but not least, we are grateful to Ilse Putman, Constance Seymour, and Judy Calabrese, staff persons in the NIST Standard Reference Data Program, for their efforts in the computer transfer and format manipulation of this monograph from the submitted computer files.

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Heat Capacity of Liquids: Volume 1
Critical Review and Recommended Values

Heat Capacity of Liquids: Volume I
Critical Review and Recommended Values

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This monograph contains recommended data on liquid heat capacities for over 1600 pure, mostly organic compounds that have melting temperatures below 573 K. The data were obtained by critical evaluation of calorimetrically measured heat capacities published in the literature. The introductory part of the monograph includes a discussion of the liquid heat capacity as a thermodynamic quantity, a brief survey of relevant calorimetric techniques, and a description of a procedure adopted for data treatment. The bulk of the monograph consists of tables for individual compounds which include information on experimental sources, the selection process, quality of correlation, and recommended data. Recommended data are presented as parameters of a correlating equation that expresses the dependence of the heat capacity on temperature, and in tables at several equally spaced temperatures. An estimate of the overall uncertainty of the recommended data is also given. At the end of the monograph, a formula and name index is provided as well as a bibliography.

Key words: bibliography; correlating equations; critically evaluated data; heat capacity; liquids; recommended values.

1. Introduction

Heat capacities belong among the basic thermophysical and thermodynamic properties which characterize a liquid. They are directly linked with temperature derivatives of basic thermodynamic functions and are therefore indispensable for the calculation of differences in these functions between different temperatures. This information is widely used in chemical engineering for establishing energy balances, in thermodynamics for obtaining entropy and enthalpy values, and in thermochemistry for calculating changes in reaction enthalpies with temperature. A knowledge of heat capacities is also required for evaluating the effect of temperature on phase and reaction equilibria. Variations in heat capacities serve as a sensitive indicator of phase transitions and are an important tool for understanding changes in the structure of liquid solutions.

1.1. Heat Capacity Calorimetry for Liquids; from the Early Measurements to the Present Status

Heat capacities were among the first physico-chemical quantities obtained by calorimetric measurements. For a number of chemicals, the first determinations were made in the 19th century using a Dewar flask as a simple drop calorimeter. As the temperatures of an ampoule with a sample and the water inside the flask differed considerably, this technique yielded enthalpy differences rather than values corresponding to true heat capacities. Other approaches were also considered, but these suggestions were more of a theoretical than practical character; the technical means available in the 19th century did not allow for the development of more sophisticated methods. The principle of relative calorimetric measurements was first mentioned as early as 1845 when Joule proposed the comparison of a sample under investigation with a well known reference substance (*45JOU) (See Sec. 6.3.1. for definition of reference format.). The first isoperibol calorimeters appeared after 1900 (02GAE); major contributions were due to Eucken (09EUC) and Nernst (10NER, 11NER), Nernst was the first to use the isothermal shield (14NER/SCH). This type of instrument ("Nernst calorimeter") made it possible to perform measurements with temperature increments of several kelvin. These were the first results which could be considered as true heat capacity values.

The most important step in the development of instruments for heat capacity measurement was the introduction of adiabatic calorimetry. This technique became widely utilized shortly after the description of the first instrument using an adiabatic jacket (20COH/MOE). Since then, a great number of such instruments have been constructed. This method achieved a high degree of sophistication and became the most important and accurate tool for heat capacity determination over a wide range of temperatures. The years between 1935 and 1970 were the most fruitful concerning both the quantity and quality of the published data; the error of high-precision measurements decreased to 0.05 percent. Most determinations were performed for condensed phases over the temperature range from several kelvin to room temperature and permitted the calculation of the absolute entropy, enthalpy, and Gibbs function at 298.15 K.

Although the accuracy of adiabatic calorimetry has not been surpassed so far, several other approaches to heat capacity measurement have been developed which are less costly, faster, and easier to use. Calculations of heat capacity from heating or cooling curves became wide-spread especially in the high-temperature region; an alternative approach was the introduction of the differential thermoconducting calorimeters. The latter concept was applied successfully in the development of commercial instruments for differential thermal analysis and differential scanning calorimetry, and has been routinely used for determining heat capacities. Recently, a significant amount of data have been generated from differential flow calorimeters which were used extensively for measurements near room temperature. Adiabatic calorimetry has not undergone any major changes or experienced new developments. The main area of change or progress has been in the high degree of automation of process control and in the introduction of microcomputers for logging, retrieval, and processing of data.

Over the past twenty years, heat capacities of liquid organic mixtures and of electrolyte and nonelectrolyte aqueous solutions have been intensely investigated near ambient temperatures; the number of systems studied largely outnumbered measurements with pure substances. This occurred due to the arrival of the Picker differential flow calorimeter (71PIC/LED) which permits very fast data acquisition over the whole concentration range; this calorimeter is available commercially. After 1980, this principle was also successfully used for investigating liquid mixtures at high temperatures and pressures.

In recent years, little experimental activity was oriented specifically towards heat capacities of pure liquids. Low-temperature measurements have been performed primarily for solids, and often in connection with superconductivity research. Systematic studies for liquid compounds contained in coal and petroleum have been performed at the National Institute for Petroleum and Energy Research (NIPER), Oklahoma (USA) and for liquid macromolecular and organometallic compounds at the Gorkii University (USSR, now Russia). Occasionally, data for various liquids have been measured in a limited temperature interval using commercial differential scanning calorimeters. Frequent measurements on mixtures near ambient conditions yield heat capacity data for pure substances as values at the limit of a concentration range.

Several reasons led to a considerable decline in measurements on pure liquids. First, low-temperature heat capacities and the derived quantities resulting from the third law thermodynamics (S, H, and G functions) are now available for many pure liquids of theoretical and/or practical interest. Funding for low-temperature measurements which are time-consuming, laborious, and require expensive and complex instrumentation are generally scarce. Second, the available data base of experimental heat capacity values is often used for the development of group contribution methods and other estimation techniques which allow prediction of thermophysical properties for a wide variety of organic structures with a typical accuracy of 5 to 10 percent. This is satisfactory for many industrial and technological applications. Because group contribution predictions are less successful for solids, thermal

properties are more often measured on them. Third, attention is now primarily focused on determining heat capacities of mixtures which offer many more possibilities for theoretical interpretation using different statistical thermodynamic models.

1.2. Scope of the Project

The project was started under auspices of the IUPAC Subcommittee on Thermodynamic Data. Its purpose was to review the state of available knowledge on heat capacities of pure substances in the liquid state and to produce the recommended values based on the evaluation of all available experimental data. The project covered organic and inorganic compounds. The criterion for inclusion of a substance in the compilation required a substance to have a melting point below 573 K. Only well-defined compounds in the isotropic liquid state were considered. Data on compounds which existed as undercooled liquids were excluded.

In order to produce thermodynamically well-defined data, we gave considerable attention to the origin of experimental values and to the conditions of their measurements. Only calorimetric heat capacities were compiled; primarily the values measured at (or close to) the saturation line were considered. Neither enthalpic measurements on reference-fluid boil-off calorimeters nor heat capacities determined by indirect techniques (see below) were considered. In general, the raw data base comes directly from experimental measurements which have been reported in the literature. Except for a few compounds for which no other data are available, comprehensive tables, calculated values, and other secondary data sources were not included. The bulk of the literature used has been published after 1920, which marks the beginning of the development of modern low-temperature calorimetry. Measurements published previous to this time were included only if no other data sources were available in the corresponding temperature interval or if the later data were obviously doubtful. All the sources of heat capacities referenced in Chemical Abstracts up to the end of 1992 were considered. Moreover the most important journals were checked for the data up to September, 1993.

Individual steps in the project were as follows:

1. Compilation of all available heat capacity data following the criteria described above.
2. Critical evaluation of the data.
3. Correlation of the selected data as a function of temperature.
4. Generation of sets of recommended values and estimation of their accuracy.

The main output of the project is the recommended isobaric and saturation heat capacities for 1624 substances. They are presented as parameters of two different correlating equations expressing heat capacity as a function of temperature for all substances (about 80 percent) for which the values are available at several temperatures. One equation serves for accurate representation of heat capacity within the temperature limits of experimental values. Discrete heat capacity values calculated from this equation are also tabulated. Parameters of the second correlating equation describe heat capacity over a larger temperature range allowing meaningful extrapolation in the direction of the critical point. Estimates of uncertainty are given for all recommended data.

1.3. Organization of the Monograph

The monograph consists of three parts: General, Indices, and Data.

The *General* part consists of several chapters. The heat capacity of liquids is discussed as a thermodynamic quantity, the result of calorimetric measurements and object of compilation efforts; the procedure adopted in this project is described and the presentation of data in this monograph is explained.

Chapter 2 defines different types of heat capacities, demonstrates their interconnection, and gives the basic thermodynamic background. Different calorimetric approaches to the heat capacity determination are analyzed in light of the thermodynamic interpretation of results. The variation of heat capacity with temperature and possible approaches to its correlation are examined.

A brief analysis of calorimetric techniques for determining the heat capacities of liquids is given in *Chapter 3*. Terminology and criteria for classifying experimental methods adopted in this project are introduced. Thereafter, a critical outline of the main experimental approaches with examples of representative calorimeters is provided. At the end of the chapter, a table summarizes all of the calorimeters referenced in the data sources which were utilized in this compilation.

Chapter 4 is an annotated bibliography of the previous compilations and evaluations regarding heat capacities of liquids and gives some description of all important secondary sources.

All the facts on the methodology of the project and handling of data are in *Chapter 5*. Rules for compiling and evaluating information from the original sources are described together with the techniques used for selection and correlation of data. Specifications are given concerning the types of recommended data and the methods used for their determination.

Chapter 6 defines the division of substances into groups for presentation purposes; the order in which the substances are listed is specified. A guide to tables gives detailed information as to how the data and accompanying information are presented and how the tables should be read.

The part *Indices* includes one literature index denoted *References* presenting all references to literature sources. For locating a substance according to its code number, the *Formula index* and *Name index* at the end of the monograph can be used.

The bulk of the monograph is the *Data* part consisting of tables for individual substances which include information on experimental sources, selection process, quality of correlation and recommended data. All of the data for one substance are presented together in several tables along with a deviation plot. The substances are ordered into groups according to chemical structure; short introductory discussions precede each group. Each substance presented is assigned a characteristic code which determines its position inside the tables.

1.4. Summary of Notation

Note: Symbols which occur only once in the text are not listed

Symbols:

Roman letters:

A	Helmholtz energy
A_i	correlation parameters
A'	time integral of the thermopile voltage
C	heat capacity
c	specific heat capacity
d	deviation
F	volumetric flow rate
f	correction factor
G	Gibbs energy
H	enthalpy
k_e	constant of proportionality
k_{ht}	heat transfer coefficient
L	heat loss
m	number of adjustable parameters
N	amount of substance (moles)
n	number of experimental points
P	power input
p	pressure
Q	heat
R	universal gas constant
S	minimized objective function
S	entropy
s	deviation
T	temperature (kelvin)
t	temperature (°C)
U	internal energy
U_e	voltage
V	volume

Greek letters:

α	thermal expansivity
β	isothermal compressibility
γ	thermal pressure
Δ	difference function
δ	deviation
ξ	function $(1 - T/T_c)$
ρ	specific density
Σ	sum
σ	error
σ^2	variance
τ	time

Superscripts:

g	gaseous
l	liquid

Subscripts:

avg	average
amp	ampoule
b	bias
c	critical point
cv	calorimeter vessel
exp	experimental (raw) value
fi	final
i	general index
in	initial
j	general index
m	molar
nb	normal boiling temperature (p_{sat} = 101325 Pa)
p	constant pressure
r	relative; reduced
re	reference
rec	receiver
s	sample
sat	saturation curve
sm	fitted (smoothed) value
su	surroundings
T	constant temperature
t	two-phase equilibrium system
V	constant volume
v	vaporization
w	weighted

2. Heat Capacities of Liquids—Thermodynamic Background

2.1. Definitions, Basic Relationships

Heat capacity C is defined by the differential equation

$$C = (\partial Q/\partial T)_x \qquad \text{(II-1)}$$

where Q indicates the amount of heat exchanged between the system studied and the surroundings when the temperature T changes under conditions specified by x. These conditions have to be specified as the heat Q is not a state function or quantity, and C varies according to different paths along which Q is exchanged. The corresponding intensive quantities are related to the unit amount of mass — *specific* heat capacity c, or to one mole — *molar* heat capacity C_m. Sometimes, heat capacities are also denoted as *thermal coefficients*.

Several different temperature gradients of thermodynamic functions are encountered in the literature: the *isochoric heat capacity* or *heat capacity at constant volume*

$$C_V = T(\partial S/\partial T)_V = (\partial U/\partial T)_V = -T(\partial^2 A/\partial T^2)_V, \qquad \text{(II-2)}$$

the *isobaric heat capacity* or *heat capacity at constant pressure*

$$C_p = T(\partial S/\partial T)_p = (\partial H/\partial T)_p = -T(\partial^2 G/\partial T)_p, \qquad \text{(II-3)}$$

the *saturation heat capacity*

$$C_{sat} = T(\partial S/\partial T)_{sat}, \qquad \text{(II-4)}$$

and $(\partial H/\partial T)_{sat}$ and $(\partial U/\partial T)_{sat}$ which do not have any specific designation and are less common. The thermodynamic functions U, H, S, A, and G are internal energy, enthalpy, entropy, Helmholtz function, and Gibbs function, respectively. The subscript "sat" denotes derivatives along the saturation (*orthobaric*) curve. For simplification of the notation, we use throughout this monograph the symbols C_p, C_V, and C_{sat}; they are also used for denoting molar heat capacities (omitting subscript m). The connection of individual coefficients with entropy and enthalpy is illustrated schematically in Fig. 1. For plots of S versus the logarithm of T and of H versus T the slopes of isochores, isobars, and saturation line correspond directly to the quantities introduced above. While the heat capacities defined by equations (II-2) and (II-3) can relate to any combination of temperature and pressure, the other three temperature gradients are by definition confined to the saturation curve (T, p_{sat}). It should be stressed that C_{sat} is *not* identical to $(\partial H/\partial T)_{sat}$ as is sometimes expected on the basis of the mistaken analogy with equation (II-3).

Using well known thermodynamic relationships, one can derive conversion equations between the individual thermal coefficients (56HAA, 82ROW/SWI, 89MAJ/SVO):

$$\begin{aligned} C_p - C_V &= T(\partial p/\partial T)_V(\partial V/\partial T)_p \\ &= -T(\partial V/\partial T)_p^2/(\partial V/\partial p)_T \\ &= -T(\partial p/\partial T)_V^2/(\partial p/\partial V)_T \end{aligned} \qquad \text{(II-5)}$$

$$C_p - C_{sat} = T(\partial V/\partial T)_p/(\partial p/\partial T)_{sat} \qquad \text{(II-6)}$$

$$C_V - C_{sat} = -T(\partial p/\partial T)_V/(\partial V/\partial T)_{sat} \qquad \text{(II-7)}$$

$$C_p - (\partial H/\partial T)_{sat} = -[V - T(\partial V/\partial T)_p](\partial p/\partial T)_{sat} \qquad \text{(II-8)}$$

$$C_V - (\partial U/\partial T)_{sat} = [p - T(\partial p/\partial T)_V](\partial V/\partial T)_{sat} \qquad \text{(II-9)}$$

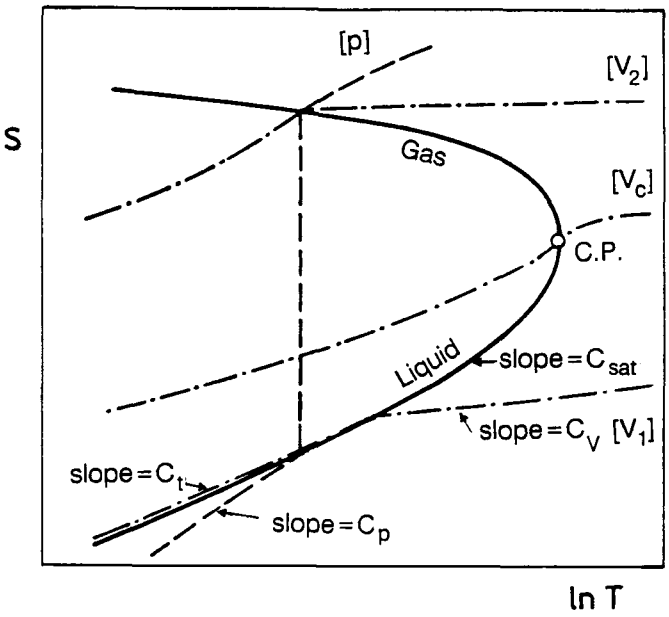
$$C_{sat} - (\partial H/\partial T)_{sat} = -V(\partial p/\partial T)_{sat} \qquad \text{(II-10)}$$

$$C_{sat} - (\partial U/\partial T)_{sat} = p(\partial V/\partial T)_{sat} \qquad \text{(II-11)}$$

where

$$(\partial V/\partial T)_{sat} = (\partial V/\partial T)_p + (\partial V/\partial p)_T(\partial p/\partial T)_{sat}. \qquad \text{(II-12)}$$

The partial derivatives on the right-hand side of equations (II-5) to (II-12) are often expressed in terms of mechanical coefficients $\alpha_p = (\partial V/\partial T)_p/V$ (*thermal expansivity*), $\beta_T = -(\partial V/\partial p)_T/V$ (*isothermal compressibility*) and $\gamma_V = (\partial p/\partial T)_V$ (*thermal pressure*) which are available for many pure liquids. The coefficient $(\partial p/\partial T)_{sat}$ is easily accessible from the temperature dependence of the vapor pressure. Below the normal boiling temperature, the term $(\partial V/\partial p)_T(\partial p/\partial T)_{sat}$ in equation (II-12) is negligible compared with $(\partial V/\partial T)_p$. Except for γ_v, all coefficients increase with



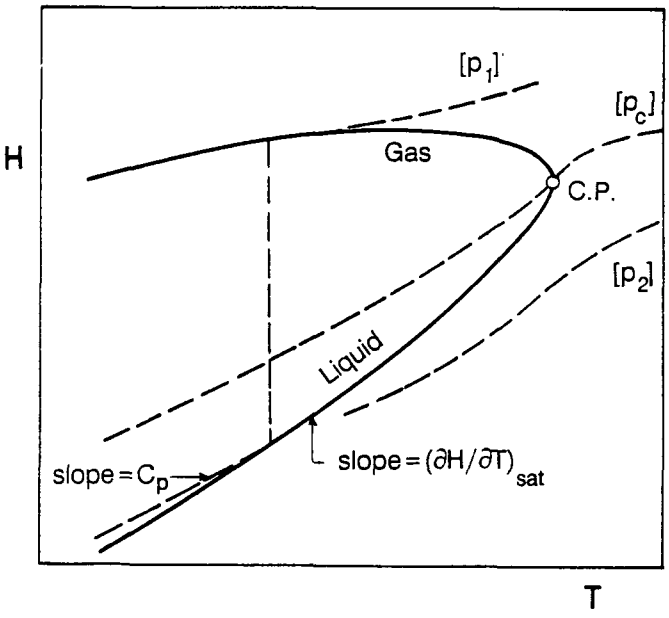


FIG. 1. Schematic plot for entropy and enthalpy of a fluid as a function of the logarithm of temperature and temperature, respectively; C_p—isobaric heat capacity, C_V—isochoric heat capacity, C_{sat}—saturation heat capacity, C_t—isochoric heat capacity of a two phase system; full lines—saturation curve, dashed lines—isobars $p_1 < p_c < p_2$, dashed-dotted lines—isochores $V_1 < V_c < V_2$, C.P.—critical point.

increasing temperature; α_p and β_T are equal to plus infinity at the critical point. For example, for liquid benzene at the normal boiling temperature ($T_{nb} = 353.3$ K), the values of the coefficients are as follows: $V_m = 9.59 \cdot 10^{-5}\ m^3 \cdot mol^{-1}$, $\alpha_p = 1.35 \cdot 10^{-3} K^{-1}$, $\beta_T = 1.52 \cdot 10^{-4} kPa^{-1}$, $\gamma_V = 8.9\ kPa \cdot K^{-1}$, and $(\partial p/\partial T)_{sat} = 3.13\ kPa \cdot K^{-1}$.

It holds for the saturated liquid that (82ROW/SWI):

$$(\partial H/\partial T)_{sat} > C_p > C_{sat} > (\partial U/\partial T)_{sat} > C_V. \qquad \text{(II-13)}$$

The first nonequality applies only when $T\alpha_p < 1$, which is the case for most liquids. The differences between the individual coefficients increase with increasing temperature and

all five are equal to infinity at the critical point. The first four quantities usually agree below the normal boiling temperature T_{nb} to within several tenths of one percent and divergence becomes more important only above that temperature. For liquids, therefore, it is not necessary to make any clear distinction below ~0.9 T_{nb} between C_p at the saturation curve and C_{sat} as the differences are less than the uncertainty obtainable in high precision measurements. For instance, a difference of 0.1 percent between C_{sat} and C_p is observed for benzene at 333 K, and the same difference for n-heptane and water, is observed at 358 and 403 K (T_{nb} = 371.6 and 373.2 K), respectively.

The differences between C_V and the other coefficients are more important at all temperatures. For example, for liquid benzene and n-heptane, C_p and C_V differ by 40 and 50 $J \cdot K^{-1} \cdot mol^{-1}$ near their respective T_{nb}. The typical variation of C_p, C_V, and C_{sat} with temperature for n-heptane is depicted in Fig. 2. It should be stressed that the above inequality does not generally apply to the saturated gas where C_{sat} can assume negative values for small molecules. Corresponding heat capacities for gases are always lower when compared with those for liquids.

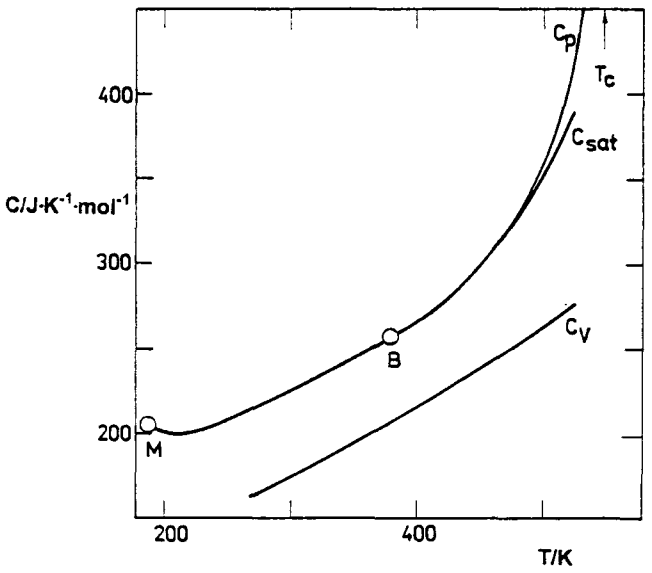


FIG. 2. Temperature variation of C_V, C_p, C_{sat} for n-heptane (according to 82ROW/SWI) M—melting temperature, B—normal boiling temperature, T_c—critical temperature, C_p—isobaric heat capacity, C_V—isochoric heat capacity, C_{sat}—saturation heat capacity.

Data on C_p and C_V are often available at conditions removed from the saturation curve. The variation of these coefficients with pressure and volume, respectively, is expressed by the differential equations:

$$\left(\frac{\partial C_p}{\partial p}\right)_T = -T\left(\frac{\partial^2 V}{\partial T^2}\right)_p \qquad \text{(II-14)}$$

$$\left(\frac{\partial C_V}{\partial V}\right)_T = T\left(\frac{\partial^2 p}{\partial T^2}\right)_V \qquad \text{(II-15)}$$

which can be used for the conversion of the data to saturation conditions. By integration, one obtains the relationships:

$$C_p(T, p_{sat}) - C_p(T, p) = -T\int_p^{p_{sat}} (\partial^2 V/\partial T^2)_p \, dp \qquad \text{(II-16)}$$

$$C_V(T, V_{sat}) - C_V(T, V) = T\int_V^{V_{sat}} (\partial^2 p/\partial T^2)_V \, dV \qquad \text{(II-17)}$$

where V_{sat} is the molar volume at T and p_{sat}. The conversion between the two states can be performed provided the *pVT* data for the liquid are available.

There are two principal methods for the determination of the heat capacities of liquids. The first method is an *indirect* approach and consists in the calculation from the other properties which are available experimentally. This approach utilizes the thermodynamic relationship of heat capacities to the combinations of different mechanical and adiabatic coefficients which can be obtained from *pVT* and speed of sound measurements. The calculations are easy, but not very accurate, and results with an error below one percent can rarely be obtained. Indirect determinations have not yielded a significant number of results because the input data are available only for a limited number of substances. This method is described by Cruickshank and coauthors in 68MCC/SCO. In compiling data for this monograph, we did not consider any heat capacities obtained by indirect methods.

The second method consists of *direct* determination by a calorimetric measurement. The thermodynamic and methodological aspects of this approach are discussed briefly below.

2.2. True and Average Heat Capacity

In most calorimetric measurements, a sample under investigation is heated or cooled and the quantity measured is the amount of exchanged heat corresponding to a finite temperature change. The *true* heat capacity is, however, a differential quantity and the experimental value obtained as the ratio of heat and temperature increment cannot be automatically considered as C in equation (II-1). It is rather the *average* heat capacity, C_{avg}, defined as the amount of heat necessary to change the temperature of a system by one kelvin. The average heat capacity is expressed by:

$$C_{avg} = \frac{Q}{(T_2 - T_1)} \qquad \text{(II-18)}$$

in an interval defined by the temperatures T_1 and T_2. This value is related to the average temperature, $T_{avg} = (T_1 + T_2)/2$.

The relationship between C and C_{avg} is obtained by introduction of the integrated equation (II-1) into equation (II-18):

$$C_{avg} = \frac{1}{(T_2 - T_1)}\int_{T_1}^{T_2} C \, dT. \qquad \text{(II-19)}$$

The heat capacity of a liquid always changes with temperature and C and C_{avg} are identical at T_{avg} only when heat

capacity is a linear function of temperature. The two quantities approach each other when the temperature interval over which the average heat capacity is determined converges and they are equal to each other in the limit:

$$C = \lim_{T_1 \to T_2} C_{avg}. \qquad \text{(II-20)}$$

We find that the heat capacity of most liquids changes moderately with temperature without a strong curvature (except in the region of high vapor pressures) and the true heat capacity agrees in most cases with the experimental value within the error of measurement provided the temperature interval is not too large (intervals up to 10 K are usually acceptable). Sometimes it is preferable to proceed with a wider temperature increment in order to reduce the time of experiments.

When the $C = C(T)$ function is nonlinear and the temperature steps are too large, it is possible to apply a *curvature correction*. Three methods have been described in the literature (68MCC/SCO):

a. The heat capacity can be expanded around T_{avg} by means of a Taylor series using the terms up to T^3.

$$C = C(T_{avg}) + \left(\frac{\partial C}{\partial T}\right)\delta T + \left(\frac{\partial^2 C}{\partial T^2}\right)\frac{\delta T^2}{2} + \left(\frac{\partial^3 C}{\partial T^3}\right)\frac{\delta T^3}{6}, \qquad \text{(II-21)}$$

where all derivatives are taken at T_{avg} and $\delta T = T - T_{avg}$. After introduction of (II-21) into (II-19) and transformation of the integration variable we obtain:

$$C_{avg} = \frac{1}{(T_2 - T_1)} \int_{\frac{1}{2}(T_1 - T_2)}^{\frac{1}{2}(T_2 - T_1)} C\,\mathrm{d}(\delta T) = C(T_{avg}) + \left(\frac{\partial^2 C}{\partial T^2}\right)\frac{(T_2 - T_1)^2}{24}. \qquad \text{(II-22)}$$

The second temperature derivative of C can be obtained in an iterative way using the $C_{avg} = C_{avg}(T)$ function as the first approximation and repeating the calculation until the $C = C(T)$ values do not change.

b. The difference between C and C_{avg} is usually small and with minimal temperature dependence over the interval between T_1 and T_2. Hence:

$$(C - C_{avg})(T_2 - T_1) = \int_{T_1}^{T_2} (C - C_{avg})\mathrm{d}T =$$

$$C_{avg}(T_2 - T_1) - \int_{T_1}^{T_2} C_{avg}\,\mathrm{d}T \qquad \text{(II-23)}$$

where values of $C_{avg}(T_1)$ and $C_{avg}(T_2)$ can be obtained numerically or graphically from the $C_{avg} = C_{avg}(T)$ curve at the temperatures T_1 and T_2. This procedure can serve the experimentalist as a quick test to find out if the correction for curvature is needed.

c. If the average heat capacities are available at several temperatures and the true heat capacity as a function of temperature is described by a polynomial then by combining Eqns. (II-19) and (II-28) we obtain:

$$C_{avg} = \frac{1}{(T_2 - T_1)} \sum_{j=0}^{m} \frac{A_j}{j+1}\left(T_2^{j+1} - T_1^{j+1}\right), \qquad \text{(II-24)}$$

where parameters A_j are adjusted by least squares fitting. This method was used for correcting average heat capacity data by Wilhoit and coworkers (85WIL/CHA).

2.3. Calorimetric Determination of Heat Capacities

From the experimental point of view the individual heat capacities defined by equations (II-2) to (II-4) differ by the paths along which the heat is exchanged between the sample and its surroundings. C_V and C_p can be obtained directly by measuring with a liquid sample at constant volume and pressure, respectively. C_{sat} can be derived from measurements at constant volume using a sample in a vessel containing small vapor space. These experiments are briefly characterized below.

2.3.1. Isochoric Measurements Without Vapor Space

Isochoric measurements with liquids are difficult to carry out at temperatures far below the critical temperature where the thermal pressure coefficient, γ_V, of the liquid is large and when it is difficult to prevent any changes in the volume of the vessel. The vessel has to be constructed from a highly rigid material with a considerable wall thickness. This latter requirement has as a consequence an unfavorable ratio in the overall heat capacities of the sample and the vessel which leads to a decrease in sensitivity. The measurements at low reduced temperatures are, therefore, rare and C_V is usually calculated from the other types of heat capacity measurements via equations (II-5) and (II-7). Direct determination of isochoric heat capacities is feasible close to the critical region where γ_V is substantially smaller than that in the region remote from the critical point (61GOO).

2.3.2. Measurements at Constant Pressure

The isobaric heat capacity of a liquid can be measured directly at pressures above the saturation vapor pressure. Although the direct determination of C_p at the saturation line is not feasible, it is possible to obtain experimental values close to the conditions of vapor-liquid equilibria and to correct them by equation (II-16). Direct measurements are easy to carry out in a flow calorimeter where the liquid is pumped through the system under a pressure maintained constant by means of a controller connected in series after the instrument. This approach was recently used extensively for studying isobaric heat capacities of mixtures in a wide range of temperatures and pressures.

Determination of C_p in a batch calorimeter is much less convenient; it is necessary to conceive of a calorimetric vessel which would allow its volume to change continuously during heating in order to allow for expansion of the liquid sample under isobaric conditions. Several variations of batch calorimeters were reported in the literature; due to numerous technical difficulties, only a limited amount of data was obtained by this technique. Aqueous solutions at elevated

pressures were investigated by using a cylindrical vessel closed with a sliding piston (55GUC/CHR). Another experimental approach was the placement of a flexible metallic diaphragm at the top and/or bottom of the vessel (61BRO/FOC, 55TOD); a limited change of the internal volume is permitted in this way. When expansion occurs the pressure is not quite constant and correction *via* equation (II-14) is necessary if the temperature range of measurement with one filling is important. A more dependable alternative is to accommodate the interior of the calorimeter vessel with a highly compressible capsule as a reentrant well (64TIM, 68REC1); for instance, a flexible metal bellows made of brass or phosphoric bronze can be used. In this way, the internal volume of the vessel is substantially reduced and measurements over as much as 100 K can be performed with one filling without any serious pressure increase. Temperature inhomogeneities due to insufficient mixing of the liquid can arise. Rastorguev et al. (75RAS/GRI) used a steel calorimetric vessel connected through a metallic capillary to a large volume tank filled with argon for maintaining isobaric conditions. The effective quantity of sample in an experiment was calculated by considering the amount of liquid expelled from the calorimeter and the thermal expansion of the calorimeter vessel. A similar approach was used by Coxam and coworkers (91COX/QUI).

2.3.3. Isochoric Measurements in a Two-Phase System

Examination of the plot of the entropy versus the logarithm of temperature (Fig. 1) shows that the lowest dashed-dotted line represents an entropic isochore corresponding to a subcritical molar volume. The slope of this line on the right of the intersection with the liquid saturation curve represents C_V of a liquid and on the left of the intersection represents the isochoric heat capacity of a two-phase equilibrium system C_t for which the volume of the vapor space becomes zero when the isochore crosses the saturation curve. It is clear that except for the vicinity of the critical point, C_{sat} for the liquid must be closely related to the isochoric heat capacity of this two-phase system, with the relative mass of vapor being much smaller compared with that of the liquid. This is schematically illustrated in the entropy diagram by the proximity of the two-phase isochore and the saturation curve. From the experimental point of view, it means that the saturation heat capacity is accessible through a calorimetric measurement with a vessel filled under vacuum with a liquid which fills most of the inner space and is in equilibrium with its vapor. Then, only a small correction has to be applied in order to obtain the true value of C_{sat}. This experiment is also the most effective way to determine C_p at the saturation line (correction using equation (II-6) has to be applied when necessary). Isochoric measurement with a two-phase system is much easier to perform compared with isochoric or isobaric measurements with the liquid phase only. Most heat capacities for pure liquid substances reported in the literature were determined by this procedure. The overall heat capacity of such a two-phase system C_t consists of the contribution from the saturation heat capacities of the liquid and vapor and further reflects the heat absorbed or evolved during vaporization or condensation inside the vessel. When the temperature increases, the liquid expands and the mass transfer between the coexisting phases is necessary for maintaining equilibrium conditions. Typically, the amount of substance in the vapor space increases first, attains a maximum, and then decreases finally towards zero (under the condition that the vessel was filled in such a way that there is no vapor space at the maximum temperature).

The relationship between C_{sat} and C_t can be derived as follows (46HOG, 82ROW/SWI). The differential of the entropy of a two-phase equilibrium system S_t containing N moles of a sample can be written as:

$$dS_t = N dS_m^l + d\left[N^g (S_m^g - S_m^l)\right]. \qquad \text{(II-25)}$$

S_m^g and S_m^l are the molar entropies of the coexisting phases and N^g is the amount of substance in the vapor space which can be expressed from the total vessel volume V and molar volumes of the coexisting phases as $N^g = (V - NV_m^l)/(V_m^g - V_m^l)$. By taking the temperature derivative of equation (II-25), the saturation heat capacity of the liquid can be expressed as:

$$\frac{C_t}{N} = C_{sat} + \frac{T}{N}\left[\frac{\partial\left(\frac{\Delta S_v}{\Delta V_v}[V - NV_m^l]\right)}{\partial T}\right]_{sat} \qquad \text{(II-26)}$$

where $\Delta S_v = S_m^g - S_m^l$ and $\Delta V_v = V_m^g - V_m^l$ are the molar entropy and molar volume of vaporization, respectively. Equation (II-26) can be rearranged with use of the Clapeyron equation $(dp/dT)_{sat} = \Delta S_v/\Delta V_v$ to a more convenient form:

$$C_{sat} = \frac{C_t}{N} + T\left(\frac{\partial p}{\partial T}\right)_{sat}\left(\frac{\partial V_m^l}{\partial T}\right)_{sat} - T\left(\frac{V}{N} - V_m^l\right)\left(\frac{\partial^2 p}{\partial T^2}\right)_{sat}. \qquad \text{(II-27)}$$

The correction on the right hand side of this relationship can be easily calculated from the vapor pressure equation and pVT properties of the liquid (except when in or near the critical region, $(\partial V_m^l/\partial T)_{sat}$ is close to the isobaric thermal expansivity α_p – see equation (II-12)). The temperature variation of the two terms of equation (II-27) is illustrated for benzene in Table 1. The first term must always be positive and increase with temperature; the second term has the opposite sign as the vapor pressure is a convex function of temperature and $V/N \geq V_m^l$. The variation of the latter term with temperature is more complex in that near and below the normal boiling temperature its absolute value increases with temperature when the vapor space volume is appreciable. Thereafter, it passes through a maximum, and finally drops rapidly towards zero when the vapor space vanishes. In this limit, equation (II-27) becomes identical with equation (II-7). If the vessel is completely filled with a liquid near the upper temperature limit there is typically a temperature at which the correction terms compensate and $C_t = C_{sat}$. Table 1 shows that at temperatures below T_{nb} the overall correction never exceeds 0.1 percent and it should be considered only for high precision measurements. It can play, however, quite an important role during high pressure measurements at saturation conditions.

TABLE 1. *Correction terms in equation (II-27) for benzene;* $V_{vap} = 100(V - NV_m^l)/V$ *denotes the percentage of the vessel volume occupied by the vapor,* $I = T(\partial p/\partial T)_{sat}(\partial V_m^l/\partial T)_{sat}$, $II = -T(V/N - V_m^l)(\partial^2 p/\partial T^2)_{sat}$, $Corr = 100(C_{sat} - C_l/N)/C_{sat}$ *denotes the overall percentage difference between* C_{sat} *and* C_l/N

T/K	V_{vap}/%	C_{sat}[a]	I	II	Corr/%
		$J \cdot K^{-1} \cdot mol^{-1}$			
278. 15[b]	11.4	131.88	0.007	−0.035	−0.02
293. 15	9.8	134.87	0.015	−0.054	−0.03
313. 15	7.6	139.27	0.036	−0.079	−0.03
333. 15	5.1	144.22	0.075	−0.088	−0.01
353. 15	2.7	149.31	0.139	−0.069	0.05

[a] recommended values of C_{sat} from this compilation

[b] extrapolation outside the temperature interval of experimental data using the quasipolynomial equation (V-12).

2.4. Variation of Heat Capacity With Temperature, Correlation Equations

Thermodynamics is limited in the exact information it provides to the temperature dependence of the heat capacity for liquids; the examples of $C=C(T)$ curves are shown in Fig. 3. Typically, the heat capacity is considered to be an increasing function of temperature though there are some substances for which the heat capacity can decrease over a certain temperature range. Heat capacities, however, always increase progressively when approaching the critical region where they are unbounded. Isobaric measurements performed at supercritical pressures by flow calorimetry indicate sharp maxima on the heat capacity curve above the critical temperature. With increasing pressure, these peaks for the supercritical fluid become less pronounced and shift towards higher temperatures.

For many substances, the heat capacity curves are flat above the solid-liquid phase transition and some of them exhibit a shallow minimum in the region above their melting temperature. This is the case for many simple inorganic compounds (e.g. AsH_3, $COCl_2$, SOF_2, PH_3, SO_2, H_2O, halogens) and some organic compounds having up to five carbon atoms in the molecule (e.g., alkenes, halogenated alkanes and alkenes, oxygenated heterocyclic compounds, sulfides, thiols). This minimum is attributed to changes in the structure of the liquid near melting conditions and is not usually pronounced. At higher temperatures, a typical monotonic increase of heat capacity is observed for most of these substance.

The temperature variation of the heat capacity can become rather complex for substances exhibiting some ordering in the liquid phase (hydrogen bonded compounds). The degree of association usually decreases with increasing temperature and this association is reflected in the shape of the heat capacity curve which can have an *S* form with an inflection point (90ZAB/RUZ). For 1-alkanols with more than two carbon atoms and some of their branched isomers, the second temperature derivative of the heat capacity is positive above the triple point (*C* curve is convex), it becomes negative in the middle part of the temperature interval (curve is concave) and finally must again become positive when the critical point is approached.

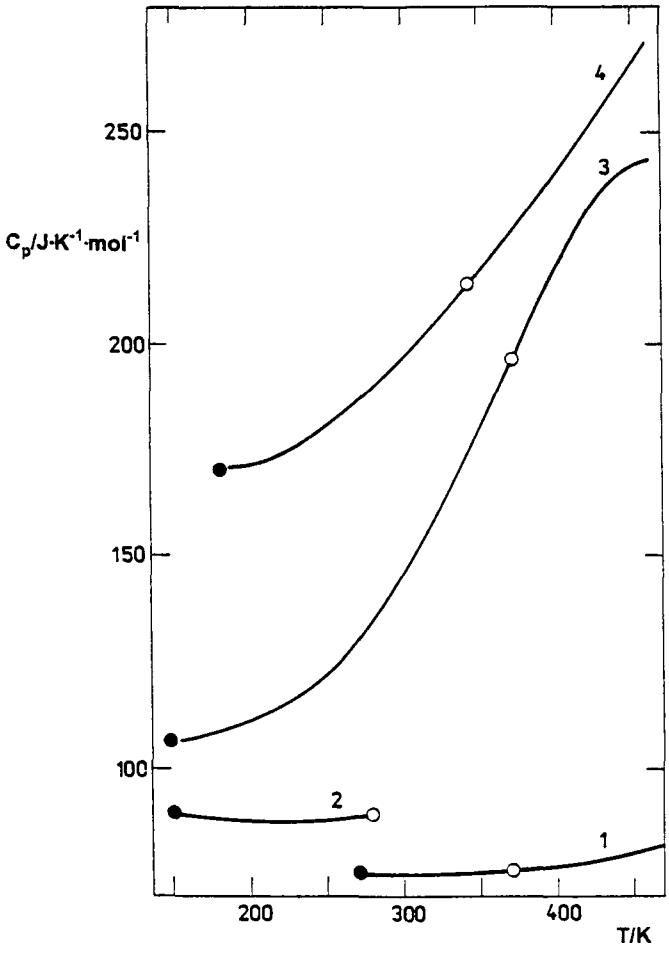


FIG. 3. Typical heat capacity curves for liquids: 1—water, temperature dependence typical for metals and simple inorganic substances, 2—methanethiol, 3—1-propanol, variation typical for 1-alkanols C_3 and higher, 4—n-hexane ● triple point temperature, ○ normal boiling temperature.

For several compounds, discontinuities (called λ-peak because of their shape) have been observed on the heat capacity curve. Such behavior was reported for instance for sulfur at 435.2 K (54BRA/MOL, 59WES1, 73KOM/MIL) and for several aldehydes (acetaldehyde at 241.9 K, 88LEB/VAS; propanal at 243 and 286 K, 77KOR/VAS; butanal at 198.2 and 284.8 K, 89VAS/LEB; hexanal at 243 K and 298 K, 91VAS/BYK). These transitions, however, did not seem to be the typical second-order phase transitions as heat exchange was observed. Little attention was paid to the explanation of these anomalies in the literature; the above cases of atypical heat capacity curves were reviewed and discussed by Zábranský at al. (93ZAB/BUR).

Empirical equations are used for correlating experimental heat capacity data. Two main criteria should be considered in selecting a relationship for fitting such experimental data:

1. The ability to describe reasonably the experimental data over the whole temperature range with a relatively small number of parameters is required.

2. The possibility of a meaningful extrapolation outside the temperature limits of experimental data is desired.

A *polynomial* seems to be the most dependable expression to describe heat capacity as a function of temperature and

has been used most often. The general form of a polynomial expression is:

$$C = \sum_{j=0}^{m} A_{j+1} T^j, \qquad \text{(II-28)}$$

where A_j are adjustable parameters and, usually, $3 \geq m \geq 1$. However, for some compounds up to eight parameters would have to be used for a satisfactory description of C over the whole temperature range where experimental data are available. A substantial drawback of a high-degree polynomial is the possibility of oscillations.

A reasonable alternative is the use of cubic splines which prove to be valuable in describing complex functions in a number of applications. Cubic splines are used in this monograph for fitting the data for some compounds. They are as flexible as high-degree polynomials without having the risk of numerical instabilities.

The principle of interpolation by cubic splines is as follows. The overall interval of the independent variable (temperature) $<T_{min}, T_{max}>$ is divided into k-1 subintervals which are delimited by temperatures $T_{min} = T_1, \ldots, T_j, \ldots, T_k = T_{max}$ called *knots*. The heat capacity as a function of temperature is approximated between the neighboring knots by cubic polynomials in temperature. The basic property of the splines is that the j-1th and the j^{th} polynomials must have at the temperature T_j not only the same values with respect to heat capacity but also must have identical values for first and second temperature derivatives. As the overall temperature range is described by k-1 cubic polynomials (each having four parameters) and the above three constraints apply to k-2 knot temperatures T_j, there are $4(k\text{-}1) - 3(k\text{-}2) = k + 2$ independent adjustable parameters. They are expressed as heat capacity values at k knot temperatures and two further constraints, typically taken as boundary conditions at T_1 and T_k. The end conditions that require the second derivative to be zero are the most common (*natural* spline).

When using cubic splines for smoothing experimental data, the knot temperatures have to be chosen first and then the heat capacity values at the respective knots are adjusted by a spline correlation routine in order to minimize the sum for squares of deviations between experimental and calculated values. The flexibility can be increased by considering the boundary conditions as two additional adjustable parameters instead of using the natural spline. It was shown (88MAJ/GAT) that spline fitting with an adjustable second-derivative end condition is equivalent to adding an arbitrary knot beyond both end knots and fitting the data with a natural boundary condition. This simplifies substantially the minimization algorithm. More specific information regarding use of splines in this monograph can be found in Section 5.3.1.

The cubic splines are very flexible when describing the temperature dependence of the heat capacity inside the limits of the temperature range of experimental data, i.e. they are excellent for interpolation. However, as with conventional polynomials, the cubic splines cannot be used for meaningful extrapolation. Thus, other formulations were used to provide reasonable extrapolations, especially towards the critical point. Engineering Science Data Unit, ESDU, Great Britain represents in its publications the heat capacities along the saturation line by expansions of the type (79ENG, 86ENG2):

$$C = \sum_{j=-1}^{2} A_j \xi^j, \qquad \text{(II-29)}$$

$$C = \sum_{j=-2}^{1} A_j \xi^{j/3}, \qquad \text{(II-30)}$$

where $\xi = (1 - T/T_c)$. Although the C values obtained from these relationships are always infinite at the critical point, there is no assurance against unrealistic behavior between the upper temperature limit of experimental data and T_c.

In this project we have used a modified version of a new type of relationship proposed by Zábranský et al. (90ZAB/RUZ) which is called the *quasi-polynomial equation*. The modified quasi-polynomial equation, even though it contains less adjustable parameters, is more flexible than the original relationship. Contrary to the original quasi-polynomial equation, the modified equation gives a positive second derivative of heat capacity with respect to temperature for the entire range from the lower temperature limit to the critical temperature. A flat area on the heat capacity curve $C = C(T)$ located above the upper limit of experimental data, that was observed for some compounds when using the original equation, has not been encountered for the modified equation.

The derivation of a quasi-polynomial equation was based on the assumption that the heat capacity is always an increasing function of temperature. As attention was focused on the extrapolation capability towards high temperatures rather than on a perfect fit of experimental data, the possible presence of a minimum on the heat capacity curve was ignored. Let us suppose that the first derivative of the heat capacity with respect to the variable $T_r = T/T_c$ has the form:

$$\frac{dC}{dT_r} = R\left(\frac{a_2}{1-T_r} + \sum_{i=0}^{m_1} a_{i+3}\, T_r^i\right)^2. \qquad \text{(II-31)}$$

The expression on the right-hand side of this equation is always positive (C must increase with increasing T_r) and can be integrated to obtain:

$$\frac{C}{R} = A_1 \ln(1-T_r) + \frac{A_2}{1-T_r} + \sum_{j=0}^{m} A_{j+3} T_r^j, \qquad \text{(II-32)}$$

A_j and a_i are adjustable parameters; A_j's are automatically constrained by equation (II-31) in such a way that the temperature derivative of the heat capacity must always be positive and equal to plus infinity at the critical temperature. When m_1 is equal to 0, then $m = 1$, and three parameters are independent; when m_1 is equal to 1, then $m = 3$, and four parameters are independent. More specific information on the use of this correlation equation can be found in Section 5.3.2.

3. Calorimetric Techniques for Determining Heat Capacities of Liquids

Calorimetry is the most frequently used method for determining heat capacities of substances in the condensed state. Several publications describe heat capacity calorimeters and attempt to introduce some system of classification. A general overview of calorimetric techniques for investigation of nonreacting systems is given in an IUPAC monograph edited by McCullough and Scott (68MCC/SCO) where the emphasis is on heat capacity measurements. The review articles by Wadsö (70WAD, 85WAD) present microcalorimetric techniques and those by Lakshmikumar and Gopal (81LAK/GOP, 82LAK/GOP) describe new modern trends in determination of heat capacities; low-temperature calorimetry was reviewed by Gmelin (79GME, 87GME). Heat capacities can be determined in a variety of calorimeters which are not specifically designed for this purpose. The majority of heat capacity calorimeters for measurements with liquids can be used also for determination with solids. On the other hand, only a small number of instruments (flow calorimeters) permit measurements with both liquids and gases (or vapors).

3.1. Terminology and Criteria for Classification of Calorimeters

There is no officially established nomenclature for describing different types of calorimeters; an attempt was made by Rouquerol and Zielenkiewicz (86ROU/ZIE) to introduce a classification of calorimeters based on heat exchange considerations, paying special attention to the dynamic behavior of calorimeters. A somewhat different terminology used in this monograph is described in this section.

That part of the calorimeter which accommodates the sample will be called the *calorimeter vessel* or *cell*. In most cases, it also contains a temperature sensing element and a resistance heater which serves either in the measurements directly or during calibration. Adjacent parts of the calorimeter which surround the vessel (jackets, shields, calorimeter block etc.) will be called the *surroundings*. The heat transfer between these two parts is, in most cases, proportional to the difference in average temperatures of the heat exchanging surfaces; they are denoted below as T_{cv} (corresponding to the calorimeter vessel) and T_{su} (corresponding to the surroundings). Heat capacity determination is usually based on recording a temperature change connected with either heating or cooling of the sample. This change can be either *intermittent* (determination of temperature increment ΔT_{cv} corresponding to the exchange of a certain finite amount of heat Q) or *continuous* (measuring the heating rate $dT_{cv}/d\tau$ corresponding to the power input $P = dQ/d\tau$). Highly automated instruments which are capable of performing measurements over a wide temperature range are called *scanning* calorimeters. For intermittent heating, the heat capacity of the calorimetric vessel with its contents C_{cv} is obtained from the relationship:

$$Q = C_{cv}\,\Delta T_{cv} + \int L\,d\tau \qquad \text{(III-1)}$$

where τ denotes the heating period, and for continuous heating, from the equation:

$$P = C_{cv}\,(dT_{cv}/d\tau) + L. \qquad \text{(III-2)}$$

The first term on the right hand side of the equations expresses the accumulation of heat in the vessel and the second term corresponds to the unaccounted heat transfer between the vessel and its surroundings. The *heat loss (leak) L* stands for the amount of energy lost per unit time. In its simplest form, the equation can be expressed as:

$$L = k_{ht}(T_{cv} - T_{su}), \qquad \text{(III-3)}$$

where the *heat transfer coefficient* k_{ht} quantifies the heat exchange across the space separating the vessel from its surroundings. In some cases, this expression can become complex because terms other than $T_{cv} - T_{su}$ can also govern the heat losses (see Section 3.2.3).

Measurements are considered as *absolute* when the amount of energy exchanged with the sample is quantified, or *comparative* (*relative*) when *calibration* is necessary for determining the value of heat capacity. Calibration can be either *chemical* using a *reference substance* of well-known heat capacity or can be *electrical* using the Joule effect to determine the response of the instruments to the introduction of an exactly known amount of heat. Corrections for heat losses are established by specific procedures that depend on the design of the instrument and the technique adopted for measuring heat capacity.

Heat capacity calorimeters can be classified according to four criteria:

1. *motion of the sample inside the instrument* (batch, flow, and drop calorimeters)
2. *mode of measurement* (stationary or dynamic conditions)
3. *temperature relationship between the calorimeter vessel and its surroundings – mode of heat transfer* (adiabatic, isoperibol, isothermal, and conduction calorimeters)
4. *number of calorimeter vessels* (single vessel and twin vessel calorimeters)

TABLE 2. Criteria codes used for classification of calorimeters

Motion of sample 1		Mode of measurement 2		Temperature relation of vessel to surroundings 3		Number of vessels 4	
batch	B	stationary	S	adiabatic	A	one vessel	O
flow	F	dynamic	D	isoperibol	I	two vessels	T
drop	D			isothermal	T		
				conduction	H		
				thermopile conduction	C		

Table 2 lists individual criteria with the codes used for characterizing calorimeters in Tables 3 and 4 and in tables with experimental values (see Section 6.3.1.). In the subsequent text, the above characteristics are briefly described. It should be kept in mind that the codes serve for a concise categorization of instruments and the adopted system of classification does not pretend to be exhaustive.

TABLE 3. Types of calorimeters used for determining heat capacity of pure liquids

Type of calorimeter	Classification 1	2	3	4	Section
Adiabatic batch calorimeters with intermittent heating	B	S	A	O	3.2.1.
Adiabatic batch calorimeters with continuous heating	B	D	A	O	3.2.1.
Isoperibol batch calorimeters	B	S	I	O/T	3.2.2.
Isoperibol flow calorimeters	F	S	I	O/T	3.2.3.
Isoperibol drop calorimeters	D	S	I	O	3.2.4.
Adiabatic drop calorimeters	D	S	A	O	3.2.4.
Isothermal drop (phase change) calorimeters	D	S	T	O	3.2.4.
Thermopile conduction drop calorimeters	D	D	C	T	3.2.4.
Measurement of heating and/or cooling curves	B	D	H	O	3.2.5.
Differential heat conduction calorimeters (TA, DTA, DSC)	B	D	H	T	3.2.6.
Differential thermopile-conduction calorimeters	B	D	C	T	3.2.6.
Special dynamic methods using pulse heating	B	D	H	O	3.2.7.

TABLE 4. Survey of calorimeters for determining heat capacity of liquids

Reference	Temp. range	Measur. accuracy	Note
Adiabatic batch calorimeters with intermittent heating			
20COH/MOE	room	medium	
24WIL/DAN	300-360 K	medium	
30SOU/AND	low	0.50 %	
33SOU/BRI	low	medium	
35AOY/KAN	low	medium	
35SAG/LAC	294-570 K	low	
37OSB/STI	373-647 K	high	also for heat of vaporization
38EUC/SCH	low	medium	
39AST/EID1	low	high	
39OSB/STI	273-373 K	high	constructed for measurement of water only
39SAG/EVA	300-370 K	2.00 %	high pressure, also for heat of vaporization
40AWB/GRI	low	medium	
41YOS/GAR	low	0.20 %	
43RUE/HUF	low	0.10 %	
44BAI/TOD	80-340 K	1.00 %	
45GUT/PIT	low	0.20 %	
45SCO/MEY	low	0.10 %	
47AST/SZA	low	high	measurement error 0.1 and 0.2 % below and above 200 K, respectively
47HUF	low	0.10 %	detailed description of improvements in calorimeter, 43RUE/HUF
47OSB/GIN	medium	0.10 %	also for heat of vaporization
47SKU	room	0.30 %	
49HOR/STO	300-500 K	0.50 %	
49STA/GUP	low	medium	
50SAG/HOU	medium and high	1.00 %	high pressure (up to 6.9 MPa)
51AST/FIN	15-300 K	0.20%	
51DOL/HET	253-573 K	low	
51EUC/EIG	medium	medium	
52ADA/JOH	low and medium	high	
53WES/HAT	250-550 K	0.15 %	
54BRA/MOE	medium and high	0.50 %	
54STR/ICK	low	0.30 %	
55DAU/MAR	20- 330 K	0.20 %	
55MAR/SMI	253-553 K	0.25 %	measurement error of 0.5 % near upper temperature limit
55PAC/PIE	low	0.10 %	also for heat of adsorption
55STA/TUP	283-373 K	1.00 %	
56COO/BAL	room	high	also for heat of solution
56POP/KOL	60-300 K	0.50 %	
57PIL	low and medium	medium	
58HIL/KRA	low	0.30 %	
58WES/GIN	303-773 K	0.10 %	
59COX/SMI	273-303 K	low	
59ONK	293-373 K	high	
60BRA/MYE	low	medium	
61FLU/LEA	2-300 K	0.50 %	also for heat of vaporization
61GOO	low	high	high pressure
61ROU	283-323 K	medium	
62KOL/SER	12-340 K	0.50 %	
63AND/COU1	low	high	
63BEN	273-343 K	high	
63FEH/SEY	medium	2.00 %	
63VAR/KOP	medium and high	1.50 %	
63ZIE/MUL	20-300 K	0.50 %	
64ARN1	293-453 K	0.30 %	
65STE/BLA	10-360 K	0.10 %	
65SUG/SEK	15-310 K	0.30 %	
66DWO/GUI	low	2.00 %	
66FIE	low	medium	
66KLE	293-343 K	high	
66NIK/LEB	60-300 K	0.30 %	
66SHI/ATA	low	high	
67AND/COU	300-450 K	medium	
67GRO	293-1048 K	0.30 %	
67RAS/GAN	298-473 K	0.50 %	
68BAG/KUC	2-300 K	1.00 %	measurement error: 4 % at 2.6 K, 2 % at 4 K, 1 % at higher temperatures
68CLE/MEL	80-320 K	high	
68LEA	298-773 K	high	measurement error 0.1 and 0.2 % below and above 673 K, respectively
68REC1	room	medium	
68WES/FUR	low	high	
68WES/WES	300-800 K	high	
69PAU/LAV2	low	high	
71GOP/GAM	303-343 K	1.00 %	
71MAY/WAL	77-400 K	medium	
72VAN	123-373 K	high	
73SHI/ENO	low	high	

TABLE 4. Survey of calorimeters for determining heat capacity of liquids — (Continued)

Reference	Temp. range	Measur. accuracy	Note
74ATA/CHI	2-300 K	high	
74DIA/REN	medium	0.30 %	
74MOS/MOU	273-346 K	low	
75MON	12-433 K	0.20 %	
76DWO/FIG	low	medium	
76LEB/LIT	5-340 K	0.30 %	measurement error: 3-5 % below 20 K, 0.5-1 % between 20-60 K, 0.15-0.3 % above 60 K
77KU /COM	low	1.00 %	
77NAZ/MUS	293-620 K	1.50 %	high pressure (up to 50 MPa)
77VOR/PRI	room	high	
78SOL/SUK	123-283 K	medium	also for heat of vaporization
79AMI/LEB	5-300 K	high	
79SCH/OFF	90-350 K	high	
79VES/ZAB	293-318 K	0.50 %	
79ZHO/KOS	9-300 K	0.40 %	
80GUR/GAV	5-300 K	0.20 %	measurement error: 1.5 % below 12 K, 0.5 % between 12-30 K and 0.2 % above 30 K
80KAL/JED	90-300 K	0.10 %	
80SHA/LYU	15-330 K	0.50 %	
80VAS/TRE	313-623 K	low	
82KAR/IGA	medium	0.50 %	
82OGU/WAT	100-370 K	0.50 %	high pressure (up to 110 MPa)
83ANI/VOR	298-393 K	medium	
83KUK/KOR	263-353 K	0.20 %	
83TAN/ZHO	medium	high	
83YOS/SOR1	15-390 K	0.20 %	
84POD/RAC	medium	medium	
85BOU/DEL	medium and high	medium	
85RAB/SHE	low	0.30 %	measurement error: 1.8 % below 10 K, 0.8 % between 10-25 K, 0.3 % above 30 K
86DEV/GUS	low	0.20 %	measurement error: 2 % between 5-25 K, 0.5 % between 25-50 K, 0.2 % above 50 K
87KHO/BUG	low	1.00 %	soviet commercial calorimeter produced at VNIIFTRI
87VAN/VAN	10-350 K	0.20 %	
87ZAB/HYN	290-373 K	0.50 %	
88ZHA/ZOU	medium	medium	
89KHO/PUL	low	medium	
89KON/STR	low	medium	
91SVO/ZAB1	293-353 K	0.30 %	also for heat of vaporization
Adiabatic batch calorimeters with continuous heating			
31DEE	low	medium	
51POP/GAL	300-1000 K	medium	64VAS2203-423 K0.50 %
65FIN/GRU	room	0.40 %	
71MUS	293-773 K	2.50 %	high pressure (up to 50 MPa)
75RAS/GRI	medium and high	1.00 %	high pressure
87OKH/RAZ	medium	0.30 %	
88LUS/RUB	14-300 K	0.05 %	
Isoperibol batch calorimeters			
07BAT	low	low	
09SCH	medium	low	
12SCH1	medium	low	
14GRI	medium	low	
16EUC	low	low	
19DEJ	medium	low	

TABLE 4. Survey of calorimeters for determining heat capacity of liquids — (Continued)

Reference	Temp. range	Measur. accuracy	Note
20GIB/LAT	low and medium	low	
21JAE/VON	room	medium	
23SIM/LAN	low	medium	
24EUC/KAR	low	0.60 %	
24KEY/BEA	low and medium	1.00 %	also for heat of vaporization
25DRU/WEI	room	low	
25PAR	low	0.50 %	
26DAN/JEN	low	2.00 %	
27FER	medium	low	
28EUC/HAU	low	low	
28GIA/WIE1	low	0.20 %	
28LAT/GRE	low	medium	
29CLU1	low	medium	calorimeter vessels, one glass and one metal
29KEL1	low	medium	
29MIT/HAR1	low	medium	
30CAR/STO	303-773 K	medium	
30WIE/HUB	low	medium	
31BLA/LEI	medium and high	3.00 %	
31FIO/GIN	medium and high	high	also for heat of vaporization
31FOR/BRU	medium and high	low	
32NEU	medium	medium	
33LEB/MOE	room	medium	
33POH/MEH	medium	low	
34KOL/UDO2	room	low	differential instrument
35JAC	medium	medium	
35KEE/KEE	low	medium	
36AST/MES	low	medium	
36CLU/GOL	low	medium	
36GIA/STO	low	0.20 %	
36PEA/BAK	low	medium	
37ELL	medium	medium	
37GIA/EGA	low	high	measurement error: 3 % at 15 K, 1 % at 20 K, 0.2 % above 35 K
37KAN	low	medium	
37PER1	low	0.40 %	
37VOL	room	low	
38HIC	low	0.30 %	
38KAI	low	0.40 %	
39BYK	298-305 K	low	differential instrument
39MAZ3	low and medium	low	
39RIE3	low	1.00 %	
40BEN/MCH	medium	low	
40CLU/POP	low	medium	
41GIA/MEA	low	high	
41NEL/NEW	273-333 K	0.50 %	
43BAC/PER	medium	medium	
48TSC1	room	low	also for heat of mixing
49TSC/RIC1	room	medium	also for heat of mixing
49WEI	room	low	
50JOH/CLA	low	high	
50URA/SID	medium	1.00 %	
51HUL/WIL	low	0.50 %	
51PAR/SIM	low	medium	adiabatic conditions below 190 K
52STA/AMI	medium	low	also for heat of vaporization
53LLE	medium	1.00 %	
53RIF/KER	low	medium	high pressure (up to 3.5 MPa)

TABLE 4. Survey of calorimeters for determining heat capacity of liquids — (Continued)

Reference	Temp. range	Measur. accuracy	Note
54OSB/ABR	low	5.00 %	
54ROB/SYD	low	high	
55HUT/MAN	297-299 K	medium	
55RUI1	room	medium	also for heat of mixing
55TAY/JOH	low	0.30 %	
56MUR/VAN	room	2.35 %	
57CRU/JOS	medium	2.00 %	
57HAR/MOE	medium	0.50 %	
57HIL/LOU	low	1.00 %	
57KEN	medium	1.00 %	also for heat of mixing
58CHE	low and medium	low	
59BAK	300-353 K	high	
60BAR/BOL	293-533 K	5.00 %	
61EGA/LUF	room	medium	
62KAT	medium	medium	
64KRO/VEN	medium	medium	
64MOE/THO	293-313 K	low	
64RAS/BAS	medium	1.50 %	
66DRA/LAN	room	medium	
66SAV	293-333 K	1.20 %	
67GRA	303-338 K	1.00 %	
69STO/MAR	room	low	for heat of mixing
69TOM/LIN	room	low	
70LKB/COM	278-333 K	medium	
70REC	room	medium	
75PED/KAY	medium	1.00 %	
76BON/CER	room	medium	
76GIE/WOL	low	3.00 %	
78RYB/EME	medium	low	
79CZA	room	low	high pressure (up to 1000 MPa)
80FUC	293-300 K	0.50 %	
86KAU/HEI	room	low	
88ROD/MAR	room	medium	commercial instrument Tronac model 458
89VAS/NOV	medium	low	
Isoperibol flow calorimeters			
23JEN/SHO	medium	medium	
28LAN	*medium*	*medium*	
31FOR/BRU	high	2.00 %	
59RIB/EGO	293-573 K	medium	high pressure (up to 25 MPa)
65KAU/BIT	293-350 K	1.00 %	
68AHL/YOU	medium	2.00 %	heat exchanger (cooling water)
71PIC/LED	room	medium	diff. instrument, comm. version SETARAM, SODEV
75SAF/GER	medium and high	0.60 %	high pressure (up to 50 MPa)
75SAN	293-573 K	0.60 %	high pressure (up to 5 MPa)
79VAN/ZEL1	100-300 K	1.00 %	high pressure (up to 7 MPa)
83GOR/SIM	medium	medium	
85OGA	room	0.10 %	
87LAN/CRI	high	medium	
Isoperibol drop calorimeters			
*79BER	medium	low	
*81VON	medium	medium	
*85STO/WIL	medium	low	
*86LUD	medium	low	
*86SCH	medium	medium	
*92STO	medium	low	
*98LOU	medium	medium	
01KAH	medium	low	

TABLE 4. Survey of calorimeters for determining heat capacity of liquids — (Continued)

Reference	Temp. range	Measur. accuracy	Note
07GUI1	high	low	
07GUI2	high	medium	
07WAL	room	low	pure solid metal dropped into liquid sample
08BOG/WIN	medium	low	
09GOO/KAL	high	medium	
11LEW/RAN	293-663 K	low	
11POM	medium	low	
12LUS	*medium*	*low*	
13REN	288-373 K	low	
18NAR	medium	low	
20MAA/HAT	90-298 K	2.00 %	
22HER/SCH	room	low	
24GAR/RAN	medium	low	
26AND/LYN	low and medium	low	
26AUE	medium	low	
26AWB/GRI	high	low	
26MON	290-553 K	low	
26UMI	373-1523 K	low	
30WAS1	medium	2.00 %	
33ROT/MEY2	273-628 K	medium	
36KHO/KAL	298-423 K	low	
36KUR/VOS	room	low	
36NEG	medium	medium	
38FRE/HIL1	medium	1.00 %	
40KUB/SCH	high	low	
42YOU/HIL	medium	medium	
45DAV/WIE	medium	low	
47KUR	medium	low	estimated measurement error about 5 %
47PUS/FED	room	low	
50EGA/WAK	high	medium	
56SCH/HIL	high	low	
56WAL/GRA	high	medium	
58SWI/ZIE1	*medium*	*low*	
62STR/BAR	298-323 K	low	
63GAT/KRE	low and medium	low	
64CAM/NAG	medium and high	medium	
64EDI/CUB	high	medium	
69SAD/STE	medium and high	low	
69SMI/MAT	298-373 K	medium	
71BEL/HUL	*high*	*medium*	pure solid metal dropped into the same liquid metal
71MAR/CIO	300-1300 K	low	
76LEB/RYA	298-473 K	1.00 %	
Adiabatic drop calorimeters			
30BAR/MAA	medium	1.00 %	
62LEV	1273-2773 K	0.70 %	
Isoperibol drop (phase change) calorimeters			
05DIE	273-573 K	medium	Bunsen ice calorimeter
06BER	273-430 K	low	Bunsen ice calorimeter
16BRA	medium	0.40 %	Bunsen ice calorimeter
28FIS/BIL	medium and high	low	Bunsen ice calorimeter
35BAR/CLU	medium	low	Bunsen ice calorimeter
50GIN/DOU	273-1173 K	0.35 %	Bunsen ice calorimeter
51FOL/GIG	room	0.25 %	Bunsen ice calorimeter
52RED/LON	high	0.50 %	Bunsen ice calorimeter
55GIG/MOR1	medium	medium	diphenyl ether calorimeter

TABLE 4. Survey of calorimeters for determining heat capacity of liquids — (Continued)

Reference	Temp. range	Measur. accuracy	Note
Thermopile conduction drop calorimeters			
71KON/SUU	273-343 K	0.10 %	
74SUU/WAD	273-343 K	high	
85WAD	medium	high	
Measurement of heating and/or cooling curve			
*67HIR	medium and high	low	
*90PIC	medium	low	
24SHO	233-313 K	low	
26AND	low and medium	2.00 %	
31THO/PAR	293-773 K	low	
33FER/MIL	293-323 K	1.00 %	
33STR/MAL	medium	low	
37STU	90-320 K	1.00 %	
40COC/FER	room	low	
40TUR/BAR	298-1273 K	low	
41ZIE/MES	medium	2.00 %	
49WUY/JUN	medium	medium	
50KUS/CRO	medium	1.50 %	dielectric constant measured simultaneously
50YAG/UNT	high	10.0 %	
52HOF	273-523 K	1.00 %	
55SEK/MOM	medium	medium	
58LUT/PAN	323-380 K	0.70 %	
59ABA/MUS	room	low	
64VUK/RAS	medium	3.00 %	
73KOM/MIL	373-903 K	high	
79TAK/YOK	80-1100 K	1.00 %	
81ATA/ELS	room	low	
84FIL/LAU	medium	2.00 %	
86NAZ/BAS1	303-523 K	2.00 %	high pressure (up to 50 MPa)
Differential heat conduction calorimeters (TA, DTA, DSC)			
31SWI/RYB2	room	0.50 %	
38KRE	293-453 K	low	
58BRA/WAT	low	low	
59BEN/THO	room	low	
63GUD/CAM	medium	low	
65GOD/BAR	80-623 K	2.50 %	
66PER/COM	340-510 K	1.00 %	
68OST/DOB	290-473 K	medium	
69PER/COM	medium and high	low	measurement error 1 % above 200 K
71DU /COM	room	low	
73PER/COM	medium and high	low	
74DSM/COM	173-773 K	1.00 %	
75CUC1	medium and high	low	commercial instrument Du Pont 990 Thermal Analyzer with DSC module
76MET/COM	medium and high	5.00 %	
77LAG/PIE	2-300 K	1.00 %	
79DU /COM	medium and high	low	
81ARU	medium and high	1.50 %	high pressure (up to 60 MPa)
84GUS/MIR	303-523 K	2.00 %	high pressure
86CDA/COM	medium	2.00 %	
87PER/COM	medium and high	1.50 %	
89KNI/ARC	high	1.00 %	commercial instrument Perkin-Elmer DSC-2
89PRA/RAJ	318-333 K	3.00 %	
90JIN/WUN	180-750 K	1.00 %	commercial instrument TA 2100 system; error between 180-370 K is 3 %
92BAO/CAC	medium and high	low	commercial instrument TA 4000 Mettler
92KAB/KOZ	340-520 K	1.50 %	triple-heat bridge method
Differential thermopile conduction calorimeters			
70PAZ/PAZ	medium	medium	modified commercial SETARAM microcalorimeter
74PET/TER	298-475 K	1.00 %	
76CON/GIA	medium	medium	
78BYV/JAS	medium	2.00 %	
83ROU/ROU	278-368 K	high	modified commercial SETARAM microcalorimeter DSC
84HAN/HAW	85-270 K	1.00 %	modified commercial SETARAM calorimeter (model BT)
86MER/BEN	150-1100 K	medium	commercial instrument SETARAM DSC 111
89BRE/LIC	170-370 K	2.00 %	commercial SETARAM micro-calorimeter DSC 111G
91BAN/GAR	298-573 K	medium	commercial instrument SETARAM model C-80

3.1.1. Motion of the Sample in the Calorimeter

In a *batch calorimeter* the liquid is contained in a vessel anchored in the core of the calorimeter. For loading the sample, either the vessel has to be removed or a special filling device must be used; the mass of liquid is in most cases determined by differential weighing. The vessel has to provide for the expansion of the sample or a small vapor space must be preserved. In order to increase the sensitivity of the measurements, the ratio of sample and vessel heat capacities should be as large as possible. To prevent temperature gradients construction must be such that fast and uniform distribution of heat inside the vessel is achieved. The batch arrangement is the one most frequently used with instruments operating at low and ambient temperatures.

In a *flow calorimeter*, a fluid under investigation flows at a constant rate through a heated tube; heating wire is attached inside the tube along its axis or, more often, the wire is wound around the outer surface of the tube. The increase in temperature, ΔT_{cv}, is determined by comparing the readings of the thermometers before and after the heater. The *specific density* of the sample, ρ, has to be known as only the volumetric heat capacity is otherwise obtained. From measurements of the *volumetric flow rate*, $F = \mathrm{d}V/\mathrm{d}\tau$, and the *heating input*, $P = \mathrm{d}Q/\mathrm{d}\tau$, the specific isobaric heat capacity c_p can be calculated directly using the equation:

$$P = c_p \rho F \Delta T_{cv} + L, \qquad \text{(III-4)}$$

where the product $c_p \rho F$ is called *heat capacity flux*. In a batch calorimeter, T_{cv} increases with time and becomes more or less

uniform all over the vessel. In a flow calorimeter, the temperature in the heating zone increases in the direction of the fluid flow and the temperature profile is independent of time (provided the stationary state was achieved). Problems might occur due to temperature gradients in the liquid, fluctuations in the flow rate, and undetected heat leaks. In differential flow calorimeters, these problems are eliminated.

In a *drop calorimeter*, a sealed ampoule containing a sample is heated to a well defined temperature T_{in} outside the calorimeter and is dropped subsequently into a *receiver* (which replaces the calorimeter vessel) at the lower temperature T_{rec}. Depending on the design of the calorimeter, either the temperature of the calorimeter vessel T_{rec} remains constant (i.e. all the heat is transported to the surroundings), or it changes only moderately since the heat capacity of the receiver is substantially larger compared with the ampoule containing the sample. For the first case in which T_{rec} is constant:

$$C_{amp}(T_{in}-T_{rec}) = Q + \int L d\tau, \qquad \text{(III-5)}$$

and for the second case in which T_{rec} changes, it holds that:

$$C_{amp}(T_{in}-T_{fi}) = C_{rec}(T_{fi}-T_{rec}) + \int L d\tau, \qquad \text{(III-6)}$$

where C_{amp} and C_{rec} denote the average heat capacities of the ampoule containing a sample and of the receiver, respectively. The temperature T_{fi} is the final equilibrium temperature after the ampoule has been dropped. In many drop experiments, the difference between T_{in} and T_{rec} was considerable (several tens of degrees) and, therefore, only average heat capacities were usually determined; the method is not easily applicable to sluggish processes and in situations where a phase change can occur.

3.1.2. Mode of Measurement

During an experiment in the *stationary* mode, the heat capacity is determined from the electrical energy supplied and the corresponding temperature change, ΔT_{cv}, by comparison of the status of the system before and after heating. It is not necessary to monitor the sample temperature and/or the heat transfer to the vessel as a function of time. On the other hand, the measurements in the *dynamic* mode require careful monitoring of the temperature and of the heat exchanged over the whole time period of the experiment. It is apparent that all methods using continuous heating are dynamic, while methods using intermittent heating can have either stationary or dynamic character.

3.1.3. Temperature Relationship Between the Calorimeter Vessel and its Surroundings

This criterion is very important as it characterizes the mode of heat transfer between the calorimeter vessel and its surroundings. The schematic of the four basic arrangements is depicted in Fig. 4. In an ideal *adiabatic calorimeter* there is no heat exchange between the vessel and its surroundings. All the electrical energy introduced into the vessel from its resistance heater is fully contained, however, under real conditions, corrections for small deviations from the strictly adiabatic regime are usually needed. The measurements are absolute in character and calibration is not necessary; however, the heat capacity of the empty vessel has to be determined separately or two experiments (with low and high filling) have to be run. In order to maintain the adiabatic regime, the vessel is surrounded by an adiabatic jacket whose temperature follows exactly that of the vessel surface ($T_{cv} = T_{su}$): see Fig. 4a. The resistance heater of this jacket is usually controlled automatically using information from the sensor of the temperature difference $T_{cv} - T_{su}$. This temperature difference is monitored by a thermopile or two platinum resistance thermometers connected in two arms of a Wheatstone bridge.

It is difficult to keep strict adiabatic conditions over an extended period of time; during a heat capacity experiment, the temperature changes and the gradients across the heat exchanging surfaces cannot be avoided. Sometimes the temperature of the vessel is adjusted so that it is slightly higher than that of the surroundings in order to maintain a small controlled heat transfer between the vessel and its surroundings (quasi-adiabatic regime). This heat leak is determined before and after the actual temperature increase by measuring the amount of energy necessary to be supplied to the vessel to maintain a constant temperature (79VES/ZAB, 87ZAB/HYN).

In order to minimize the heat leaks, every effort is made to reduce the value of the heat transfer coefficient k_{ht} which includes contributions to heat conduction, convection, and radiation. The latter mode of heat transfer is predominant at high temperatures while the former two play important roles at low temperatures. Calorimeters are evacuated in order to suppress conduction and convection from gas molecules. The diameters of electric leads and supports are minimized to reduce the heat conduction through the solid connections and shields are used to reduce radiation. Calorimeters equipped with a system of heated and/or unheated radiation shields can be used up to a temperature of around 800 K (58WES/GIN). Discussion of the heat transfer in calorimeters can be found in the literature (68MCC/SCO). Adiabatic calorimeters are typically single-vessel instruments of the batch type and can work both in a stationary or dynamic mode.

In an *isoperibol calorimeter* (see Fig. 4b) the temperature of the surroundings is kept constant (T_{su} = const) or close to constant and the experiment is conducted in such a manner that the difference between T_{cv} and T_{su} is kept small at any time during an experiment (usually below 5 K). The vessel is insulated from its surroundings, thus enabling most of the heat introduced from the vessel heater to be contained. By measuring the drift in the temperature of the vessel before and after heating, the correction for the heat exchange with the surroundings can be calculated. Compared with the arrangement of adiabatic calorimeters, isoperibol calorimeters are easier to construct and to operate. Isoperibol instruments were used successfully, especially at low temperatures; when the inner space of the calorimeter is evacuated, the inequality of T_{cv} and T_{su} does not lead to serious heat leaks as radiation is very low in this region. A simple isoperibol arrangement is a Dewar flask with a Beckman thermometer and a heater, placed in a

thermostatted room; such a rudimentary instrument can yield data with an accuracy of around 3 percent at room temperature. Isoperibol calorimeters are typically single vessel instruments of the batch type working in a stationary regime.

In an *isothermal calorimeter*, both the calorimeter vessel and its surroundings are always at the same constant temperature ($T_{cv} = T_{su}$). In these instruments, all the heat effect in the vessel is exactly compensated by introduction or removal of the same amount of energy. Supplying energy into the vessel by *Joule heating* is used for endothermic processes, *Peltier cooling* is used for exothermic processes. In older calorimeters, the heat was absorbed by melting or vaporizing a suitable substance; the actual amount of heat was determined from the amount of substance which underwent the phase transformation. The Bunsen "ice" calorimeter is a typical example of a *phase change calorimeter* where the difference in densities of ice and liquid water serves to quantify the heat effect (see Fig. 4c). The advantage of such a calorimeter is its simplicity of construction and no need for calibration; the substantial drawback is the limitation of the temperature of the phase change. The isothermal technique has limited use in heat capacity determinations as it can be used only for measuring average heat capacities in a drop calorimeter.

As *heat conduction calorimeters* are denoted different instruments in which the heat transfer between the calorimeter vessel and its surroundings plays a crucial role in the heat capacity determination. The experiment is based on recording the change of temperature with time after introduction of a certain amount of heat to the vessel or to the surroundings. Alternatively, the energy input needed to achieve a desired rate of temperature increase can be recorded. Heating can be continuous or intermittent, heat transfer between the sample and the surroundings can be facilitated by various types of environment. Measurements are performed in a dynamic mode and are always relative; they can be carried out in a twin calorimeter or by comparing two experiments performed subsequently under identical conditions in a single vessel calorimeter. All the instruments for heat capacity determination based on recording of *heating* and/or *cooling* curves can be considered as heat conduction calorimeters.

Thermopile conduction calorimeters are a special type of heat conduction calorimeter (see Fig. 4d) based on an idea of Tian (24TIA) and developed later by Calvet and other researchers. A thermopile consisting of a large number of thermocouples (up to several hundred) permits a *controlled* and rapid transfer of heat between the vessel and a massive *calorimeter block*. As its heat capacity is, in general, much larger compared with the thermal effect in the vessel the conditions are close to isothermal (T_{su} = const., $T_{cv} - T_{su} \rightarrow 0$). The transferred heat is proportional to the voltage U_e measured at the ends of the thermopile and its recording as a function of time τ permits one to determine the overall thermal effect from the equation:

$$Q = k_e \int U_e d\tau = k_e A', \qquad \text{(III-7)}$$

where A' denotes the total area under the recorded curve representing U_e versus τ. A constant of proportionality k_e is determined through electric or chemical calibration. In the first case a heater inserted into an empty calorimeter vessel is used to determine the relationship between the recorded signal and the amount of the heat introduced. In the second case an experiment is performed with a substance (or substances) the thermal properties of which are well known. Most calorimeters use two cells housed in separate wells inside the calorimeter block. Differential connection of their thermopiles allows one to filter out most of the heat transfer which is not associated with the measured effect. This arrangement is well suited especially for studying slow or sluggish processes. Heat capacity measurements in a classical Calvet calorimeter are not very convenient as a combination of several experiments is necessary to obtain the final value of the heat capacity (56CAL/PRA). The principle of conduction through thermopiles is, however, utilized in several commercial instruments which can serve satisfactorily for heat capacity measurements (see Section 3.2.6).

3.1.4. Number of Calorimeter Vessels

Heat capacity determinations are performed either in *single vessel* or in *two vessel* (*twin*) instruments which are also denoted often as *differential calorimeters*. The single arrangement is simpler and less expensive as it is not necessary to manufacture two identical vessels. Beside the *measuring* cell where the actual thermal effect is measured, twin calorimeters have a *reference* cell which can be empty or filled with another substance; the difference in the thermal response of the two cells is directly recorded. The main advantage of twin calorimeters is the elimination of most errors due to heat losses and the minimization of perturbations which affect both cells in a similar way; this is important particularly for working with small samples and when measuring weak thermal effects (*microcalorimetry*) as well as for investigation of slow processes. An arrangement with two vessels is also more versatile as different kinds of experiments can be designed giving directly information on differences between the heat effects in the two vessels. Absolute measurements without calibration are performed more often in one-vessel instruments (e.g. adiabatic batch calorimeters) while the twin arrangement is typically used for comparative measurements (thermopile conduction calorimeters, Picker-type flow calorimeters).

However, it should be kept in mind that the reference vessel of a twin calorimeter should not be automatically associated with a reference substance. The use of the same word reference in the two contexts is only a terminological coincidence. Actually, in many differential experiments, the measuring cell is consecutively filled with a sample and with a reference substance while the contents of a reference cell does not play any important role. A reference fluid can be used also in experiments with single-vessel instruments for calibration purposes; on the other hand, an experiment can, in principal, be performed in a differential calorimeter without a reference fluid.

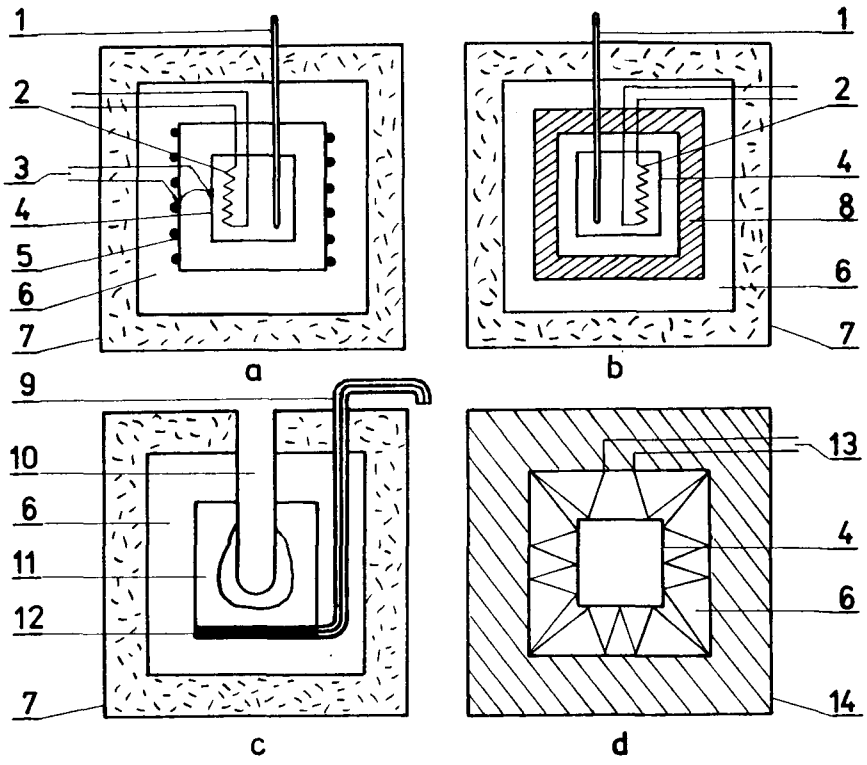


FIG. 4. Four main arrangements of calorimeters illustrating the heat transfer between the vessel and its surroundings: a. adiabatic, b. isoperibol, c. isothermal phase-change, d. thermopile conduction. 1—thermometer, 2—electric heater, 3—thermopile, 4—calorimeter vessel, 5—adiabatic jacket, 6—evacuated space, 7—outer insulation, 8—massive isothermal shield, 9—capillary filled with mercury, 10—space for dropping a sample (receiver), 11—solid-liquid equilibrium mixture of the substance used for quantifying the heat effect, 12—mercury in contact with the melting substance, 13—leads of the thermopile between the vessel and the thermostatted block, 14—thermostatted massive metallic block.

3.2. Main Experimental Approaches to Determination of Heat Capacity for Liquids

This section presents a concise overview of the most important calorimetric methods for determining the heat capacities of pure liquids with examples of several representative calorimetric designs. Most of the content of the well-known IUPAC monograph on the calorimetry of non-reacting systems (68MCC/SCO) is devoted to classical techniques of heat capacity measurements with pure condensed phases. Therefore, we shall pay more attention to the developments over the last few decades and mention some modern techniques which were not primarily designed for the investigation of pure liquids, but present an important aspect of progress in the evolution of heat capacity calorimetry.

3.2.1. Adiabatic Single Vessel Batch Calorimeters

Adiabatic instruments with intermittent heating represent the most accurate tool for determining the absolute heat capacity of substances in the condensed phases in the range from temperatures close to absolute zero up to ambient conditions. High-precision instruments can yield data with an error between 0.05 and 0.1 percent. These instruments are not, however, available commercially and the construction is both complicated and time-consuming.

With the first calorimeters of this type (20COH/MOE, 24WIL/DAN), adiabatic conditions were realized using a metallic vessel immersed in a bath whose temperature was controlled (wet shield). The advantage of such an arrangement was the possibility of active cooling. With such an arrangement the control system was, however, slow in response and was subsequently used only occasionally (35SAG/LAC, 50SAG/HOU). Dry shields made from highly conductive material (copper and brass are common) with a heating wire coiled on the outer surface of the shield were introduced by Andrews (29AND, 30SOU/AND); these have been used most often for maintaining adiabatic conditions.

Referenced below are some of the laboratories and adiabatic instruments which made a significant contribution to the heat capacity determination in the range between 5 and 320 K regarding both the quantity and quality of data (typical accuracy 0.05 to 0.3 percent above 20 K and 3.0 to 5.0 percent below that temperature): the former National Bureau of Standards (today's NIST), USA (37OSB/STI, 45SCO/MEY, 47OSB/GIN), the former laboratory of the Bureau of Mines at Bartlesville (today's NIPER), USA (43RUE/HUF, 47HUF), Pennsylvania State University, USA (39AST/EID1, 47AST/SZA, 51AST/FIN, 53AST/WOO), National Physical Labora-

tory in Teddington, Great Britain (63AND/COU1, 67AND/COU, 73MAR), University of Michigan, Ann Arbor, USA (68WES/FUR) and University at Gorkii, USSR, now Russia (66NIK/LEB, 76LEB/LIT). While few new adiabatic calorimeters have been constructed in the USA and Europe in recent years, there has been recently a good deal of experimental activity in Japan (66SHI/ATA, 74ATA/CHI; a calorimeter has been described for measurements on liquid crystals up to 390 K 83YOS/SOR1). Instruments allowing measurements at high pressures were constructed by Goodwin (61GOO); Rastorguev et al. (75RAS/GRI) and Oguni et al. (82OGU/WAT). Calorimeters with a small controlled heat leak (see Section 3.1.3) have an accuracy of heat capacity determination 0.3 to 0.5 percent (79VES/ZAB, 87ZAB/HYN).

Two examples of typical adiabatic heat capacity calorimeters (one for low-temperature measurements and the second for high temperature measurements) are given in Figs. 5 and 6. The instrument of Ruehrwein and Huffman (43RUE/HUF) is a low-temperature calorimeter designed for measurements between 10 and 320 K with accuracy around 0.1 percent. The calorimeter vessel is made of copper with an inner volume of 56 cm^3. The resistance thermometer and the resistance heater resistor are housed in the well. The vessel is suspended on thin wires of low conductivity inside an evacuated space. The temperature difference between the vessel and the brass adiabatic jacket is detected by three thermocouples. Liquid hydrogen and liquid air in the reservoirs serve for cooling down the interior of the instrument; all electrical leads are wound around the floating ring to minimize heat leaks by conduction. This calorimeter yielded an impressive number of accurate data over a period of 50 years, and a number of improvements regarding process control and retrieval of data were reported.

The instrument of West and Ginnings (58WES/GIN, Fig. 6) was designed for experiments between room temperature and 773 K. In order to prevent temperature gradients, a cylindrical aluminum block with a system of coaxial channels served as an unconventional calorimeter vessel. The central channel houses the platinum resistance standard, three other channels accommodate heating resistors and the rest contain the sample (the overall interior free volume is 70 cm^3, the diameter of the channels is 2 to 5 mm). The vessel is fixed in a heated silver ring and surrounded by a system of thin silver lids and shields which serve to minimize the radiation losses. Chromel-aluminum thermocouples are used as sensors of the temperature difference between the vessel and adiabatic surroundings which consist also of several heated silver shields and lids. Temperature is controlled automatically such that the differences between individual parts inside the calorimeter are below 0.001 K. A homogeneous atmosphere inside the calorimeter is maintained by a slow flow of carbon dioxide (1 $cm^3 \cdot min^{-1}$).

Continuous heating allows for the measurements to be carried out rapidly compared with the experiments using a classical adiabatic calorimeter; the measurements are, however, usually less accurate. In order to avoid systematic errors due to temperature gradients, it is imperative to have a very fast temperature response of the entire calorimeter vessel to heating. Also, recording or logging of the primary experimental output becomes more complicated (see Eqn. III-2) since the temperature and heating rate have to be monitored continuously. The first calorimeter of this type was reported as early as the 1930's (31DEE), but significant progress was attained only with the arrival of automated techniques for temperature control and the processing of the primary output by computer methods (88LUS/RUB). A continuous heating method adapted for high pressures was reported by Guseinov and Mirzaliev (84GUS/MIR).

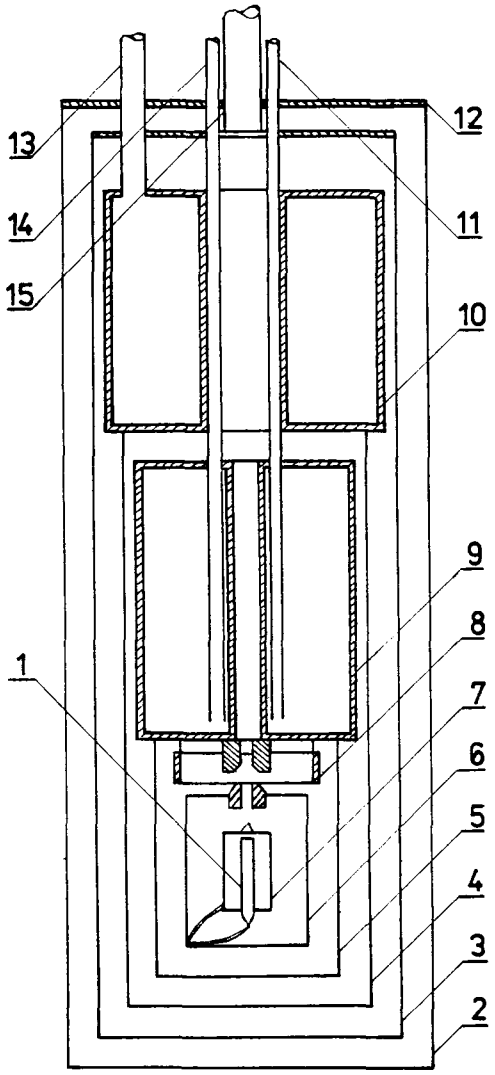


FIG. 5. Adiabatic calorimeter for low temperature measurements (43RUE/HUF)
1—well housing a heater and thermometer, 2—outer can, 3,4—copper radiation shields, 5—copper shield in contact with liquid hydrogen, 6—adiabatic jacket, 7—calorimeter vessel, 8—floating ring, 9—liquid hydrogen reservoir, 10—liquid air reservoir, 11—filling tube (hydrogen reservoir), 12—vacuum tight joint, 13—filling tube (liquid air reservoir), 14—emptying tube, 15—tube for electrical leads and connection to a vacuum line.

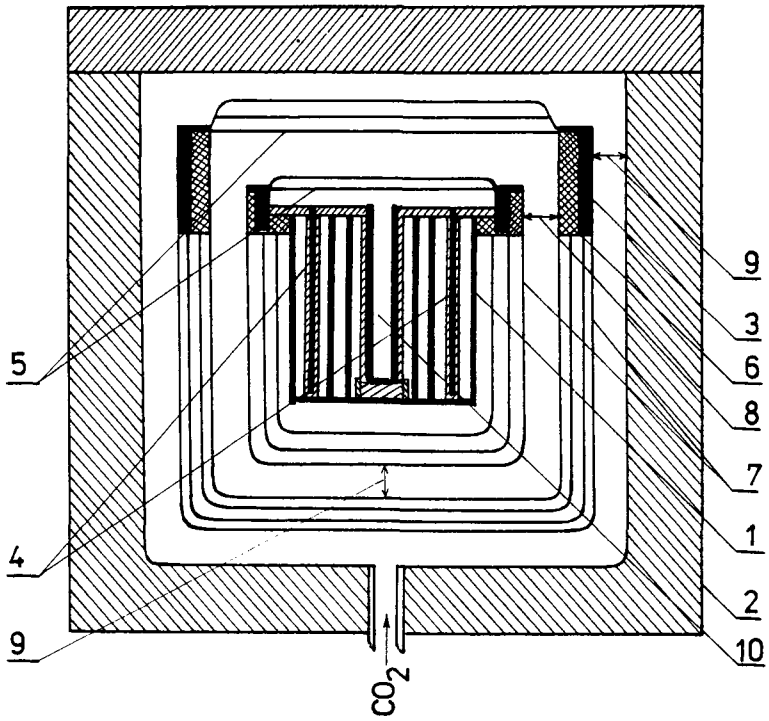


FIG. 6. Adiabatic calorimeter for high temperature measurements (58WES/GIN)
1—calorimeter vessel, 2—outer insulation, 3—heater of the adiabatic jacket, 4—vessel heaters, 5—radiation lids, 6—adiabatic ring supporting lids and shields, 7—radiation shields, 8, 9—thermocouples, 10—thermometer well.

3.2.2. Isoperibol Single Vessel Batch Calorimeters

Isoperibol calorimeters with a massive isothermal shield were frequently used for low-temperature heat capacity determination before 1940; the best measurements had an accuracy of 0.2 – 1 percent above 35 K and 5 percent below that temperature. Most of the measurements were, however, performed in simple isoperibol instruments without massive isothermal shields. Usually a Dewar vessel equipped with a thermometer and an electric heater was used (49WEI); in this case, the best accuracy which can be achieved is about 1 percent (80FUC).

Important laboratories which contributed to the development of this technique in a significant manner were University of California at Berkeley, USA (28GIA/WIE1, 37GIA/EGA) and Berlin University (29CLU1, 40CLU/POP). A typical example of this class of calorimeter is the instrument of Giauque and Egan (37GIA/EGA); its simplified scheme is depicted in Fig. 7. The calorimeter vessel is made of gold, its mass is about 500 g and the inner volume is near 170 cm^3. The platinum resistance thermometer which is calibrated using a standardized copper-constantan thermocouple is in the central well; the resistance heater is wound on the outer surface of the vessel. The measurement error is 0.2 percent except in the region of very low temperatures (see Table 4). This approach is, however, rarely used at present and is mainly of historical interest.

3.2.3. Isoperibol Flow Calorimeters

Most flow calorimeters have isoperibol character as the temperature of the surroundings is maintained constant close to the average temperature of the heated fluid. The ability to maintain a stable flow rate is the primary condition for the proper functioning of a flow calorimeter with a single cell. The first measurements on these calorimeters were, therefore, not of high accuracy (28LAN, 31FOR/BRU) and progress was achieved only with the advent of modern pumping devices. This type of instrument was successfully used for measurements at elevated pressures (75SAF/GER, 77HOF/SAN).

After the introduction of the differential arrangement was first proposed by Picker (71PIC/LED), flow calorimeters of this kind became widely utilized for measuring heat capacities of mixtures. The commercial versions of isoperibol flow calorimeters were distributed by SETARAM in Europe and by SODEV in America. Within the two last decades, a large number of measurements have been made using these calorimeters yielding much data near ambient conditions.

In a Picker calorimeter (see Fig. 8), a liquid passes through two identical cells connected in series inside a thermostatted evacuated chamber. The heating input is controlled in such a way that the temperature increase in the two cells is always identical. First the reference fluid is pumped into the system followed immediately by the sample; heating input to

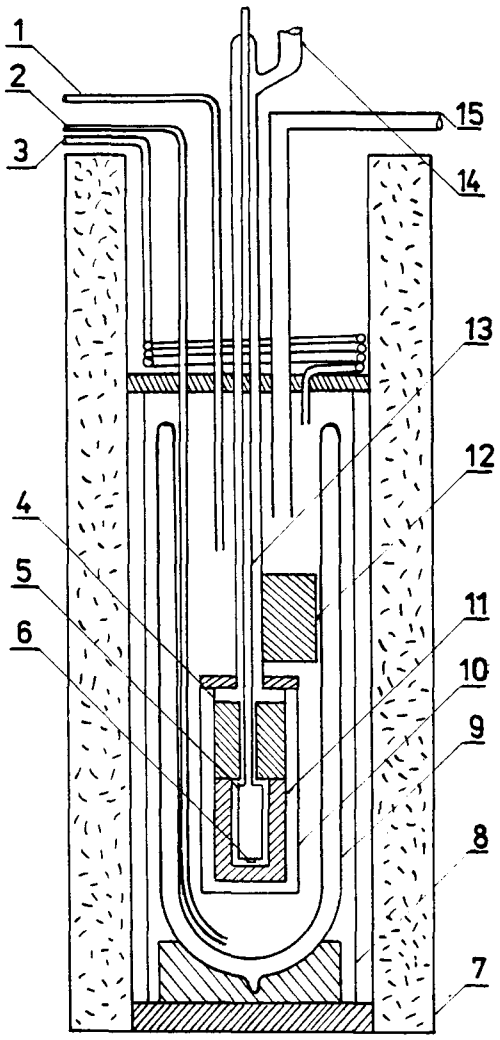


FIG. 7. Isoperibol calorimeter for low temperature measurements (37GIA/EGA)
1—transfer tube, 2—tube for removing liquid from Dewar vessel, 3—tube for introducing liquid hydrogen, 4—suspension cords for protective cylinder, 5—calorimeter vessel, 6—thermometer well, 7—outer insulation case, 8—inner case, 9—silvered Pyrex Dewar flask, 10—container of the vessel, 11—protective cylinder, 12—block for thermostatting of leads, 13—filling tube of the vessel, 14,15—vacuum lines.

the measuring cell is registered during the period when the reference fluid is present in both cells (P_{re}) and subsequently when the sample passes through the first cell and the reference fluid through the second cell (P_s). It is obvious that in such an arrangement the uncertainty due to instabilities in the flow rate are at a minimum. Experiments are rapid (about two data points in one hour) and fairly accurate (typical errors around 0.5 percent). The small diameter of the tube (inner diameter near 1 mm) reduces the risk of temperature gradients in the liquid and the amount of sample needed for an experiment (around 5 cm^3). The Picker calorimeter is not suitable for working with viscous liquids. In addition, the sample fluid must be miscible with the reference liquid of well-known heat capacity and density data for the ratio ρ_s/ρ_{re} must be available, otherwise, only heat capacities related to the unit volume can be obtained (see Eqn. III-8). Water is used as a reference for aqueous solutions and heptane is used in most cases for measurements with organic liquids.

Differential flow calorimeters are especially useful for measurements at high temperatures and pressures. It is not necessary to cool down the instrument and release the pressure for refilling. The instrument time constant is small since the volume of the cells is small, and thin-walled tubing can sustain considerable pressure. Isobaric heat capacities are directly obtained from the experiment. The absence of a vapor space or any other correction is a particular asset at superambient conditions where the correction terms are large and difficult to estimate. The first instrument of this type proposed by Smith-Magowan and Wood (81SMI/WOO) was further improved (88WHI/WOO, 91CAR/WOO) to allow measurements with corrosive fluids up to 723 K and 40 MPa (see Fig. 9). Reference liquid (water) flows first through the reference side of the calorimeter towards the six port valve. Depending on the valve's position, the reference liquid either by-passes the loop entering directly into the measuring side (base line determination) or penetrates into the loop forcing the sample into the instrument (plateau determination). Temperature equilibration to 0.01 K is secured by extensive heat exchange and a preheating system. The pressure is maintained constant to 0.02 MPa by means of two back pressure regulators connected in series. The pressure between the two regulators is utilized before the sample injection for prepressurizing the loop which is thermostatted at a well defined temperature (usually 298.15 K). This provision allows one to substitute at any temperature the ratio of sample and reference densities in Eqn. (III-8) for the density ratio at the thermostatting temperature; thus, in this arrangement, knowledge of density at only one temperature is satisfactory. During the calibration, an auxiliary pump allows the addition or withdrawal of some reference liquid before its passage through the measuring side (see below).

When Eqn. (III-4) is written for the measuring cell of a flow calorimeter for sample and reference conditions, it is easy to derive the relationship (76DES/DEV):

$$1 + f\left(\frac{P_s - P_{re}}{P_{re}}\right) = \frac{(c_p\rho)_s}{(c_p\rho)_{re}}. \qquad \text{(III-8)}$$

This equation allows one to calculate the heat capacity of the sample provided the *correction factor* f, which accounts for heat losses during experiment, is available. By comparing Eqns. (III-4) and (III-8), one finds that:

$$f = \frac{1 - \dfrac{L_s - L_{re}}{P_s - P_{re}}}{1 - \dfrac{L_{re}}{P_{re}}} \qquad \text{(III-9)}$$

where L_s and L_{re} denote heat leaks from the measuring cell.

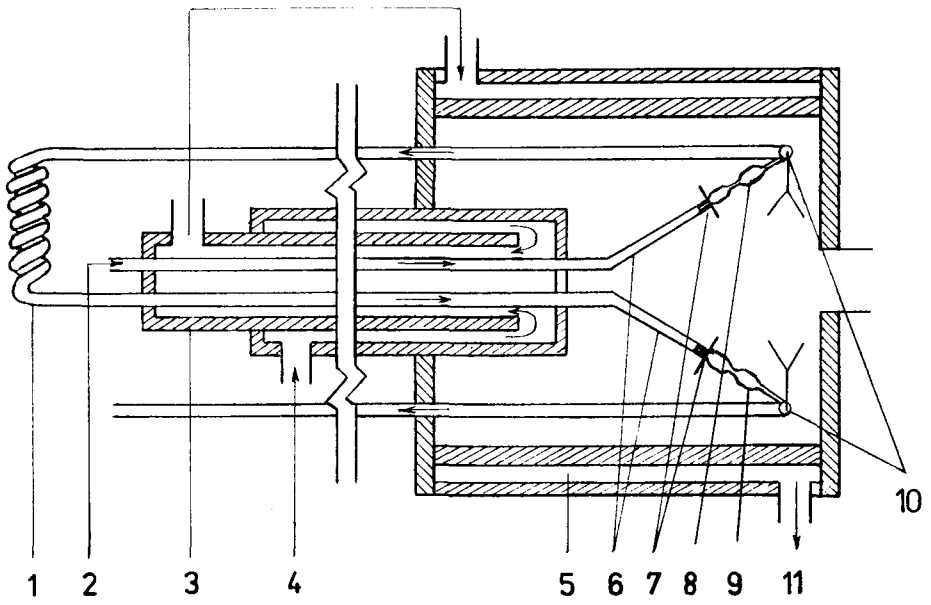


FIG. 8. Picker differential flow calorimeter (71PIC/LED)
1—external stainless steel coil, 2—injection system, 3—thermostat for injecting fluid, 4—water inlet to thermostat, 5—thermostatted water jacket, 6—stainless steel tube, 7—heaters, 8—reference cell, 9—measuring cell, 10—detector assemblies with thermistors, 11—water outlet from thermostat.

There are two methods for determining the correction factor f which in the ideal case is equal zero. The first is the measurement of ΔT_{cv}, F, and P for a fluid of well-known heat capacity and the calculation of L from Eqn. (III-4) (76FOR/BEN2, 81ROG/PIT). The second, more widespread method (71PIC/LED, 76FOR/BEN2, 81SMI/WOO, 91CAR/WOO), uses the change in heat capacity flux. Here, the change in C_p is mimicked by altering the flow rate through the measuring cell while keeping the flow rate of the same liquid through the reference cell constant. The factor f is calculated from:

$$f = \frac{P\,\Delta F}{F\,\Delta P} \qquad \text{(III-10)}$$

where ΔF and ΔP denote the change in flow rate and the corresponding adjustment of the electrical input, respectively.

In the case of a flow calorimeter, the heat losses depend on several factors; L can be expressed (82WHI/WOO, 91CAR/WOO) as:

$$L = k_{ht1}(T_{cv} - T_{su}) + k_{ht2}\frac{(T_{cv} - T_{su})}{c_p \rho F} + k_{ht3}P \qquad \text{(III-11)}$$

where the first term has the same meaning as in Eqn. (III-3). The second term expresses the heat loss due to the gradient along the tube; since temperature sensors are located at some distance from the heater, the measured ΔT_{cv} is different from the real temperature rise in the liquid due to heat exchange between the tube and its surroundings. This distortion decreases with increasing heat capacity flux. The third term represents heat losses due to the overheating of the heater on the tube surface. This term is obviously proportional to the energy input. An exhaustive analysis of heat losses and methods for determining the f factor in high-temperature flow calorimeters was published by Carter and Wood (91CAR/WOO).

3.2.4. Drop Calorimeters

In the simplest version of this technique, the interior of the Dewar flask filled with water serves as a receiver. An increase in the water temperature is measured after dropping a sealed ampoule with a sample, preheated in a furnace above the calorimeter. The actual thermal effect is calculated from Eqn. (III-6) using the calibration constant C_{rec} determined by the Joule effect or by measurement with a sample of the well known heat capacity. This rudimentary isoperibol calorimeter used to be the most widespread tool for heat capacity measurements in the 19th century; certain results were surprisingly accurate (around 1 percent, *81VON) and retain some value today. This type of experiments is denoted sometimes in the literature as the method of mixtures to express that the sample and water at two different temperatures are "mixed" to equilibrate at the third temperature. The heat capacity of the receiver is much larger compared with that of the ampoule and sample; the difference between temperatures of the furnace and the vessel must be considerable to achieve sufficient sensitivity. Therefore, "mixing" experiments give actually enthalpic differences rather than heat capacity values. Currently, this method is used only for measurements at high temperature where the heat capacities are large and do not change significantly with temperature; in this case, melted metal is used instead of water (71BEL/HUL).

Drop calorimeters were rarely run under adiabatic conditions (30BAR/MAA, 62LEV). The isothermal arrangement, in

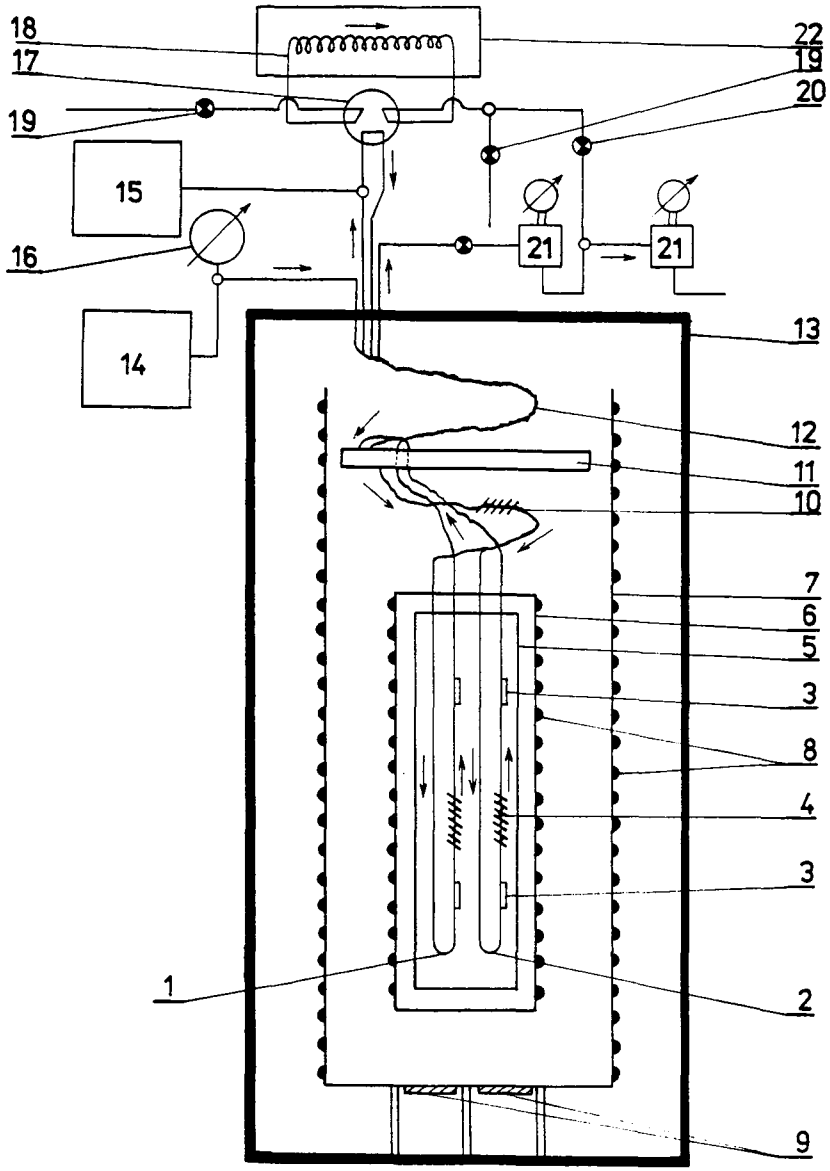


FIG. 9. Scheme of a differential flow calorimeter for measurements at high temperatures and pressures (91CAR/WOO), direction of flow is indicated by arrows
1—reference side, 2—measuring (sample) side, 3—platinum resistance thermometers, 4—heater, 5—calorimeter block, 6—inner isothermal jacket, 7—outer isothermal jacket, 8—coaxial heater cable, 9—strip heaters, 10—coaxial preheater, 11—preheater lid, 12—counter-current heat exchanger, 13—vacuum can, 14—HPLC pump, 15—auxiliary pump used for calibration, 16—pressure gauge, 17—HPLC six port valve, 18—thermostatted sample loop, 19—valves for filling the loop, 20—prepressurization valve, 21—back pressure regulators, 22—thermostat of the sample loop.

which all the heat transferred from the ampoule is "pumped out" from the receiver keeping T_{rec} constant (see Eqn. III-5), seems to be the most convenient for drop experiments. Phase-change calorimeters were often used as they are easy to construct and allow experiments to be performed under isothermal conditions without any electronic equipment. Measurements were carried out for example at the National Bureau of Standards, USA in a Bunsen ice calorimeter on a number of substances between 273 and 1173 K (47GIN/COR, 56FUR/DOU). Drawbacks of using the water-to-ice phase transition as a heat exchange indicator are the low sensitivity due to the high value of the specific enthalpy of melting for ice and the negative sign of volumetric change accompanying the melting ice. In this case, as shown in Fig. 4c, mercury is sucked inside the instrument. Diphenylether (melting temperature 300.05 K) is more suitable for use in phase change calorimeters (55GIG/MOR1), because its volumetric change at melting is positive and has a specific enthalpy of melting almost four times lower than water.

A thermopile conduction drop calorimeter for measurement with small samples below 1 g in the temperature range from 273 to 343 K was developed by Wadsö and coworkers (71KON/SUU, 74SUU/WAD, see Fig 10). Two identical ampoules can be preheated in a furnace and dropped simultaneously into the receivers of a calorimeter which is thermostatted at a working temperature about 10 K lower; the recorded

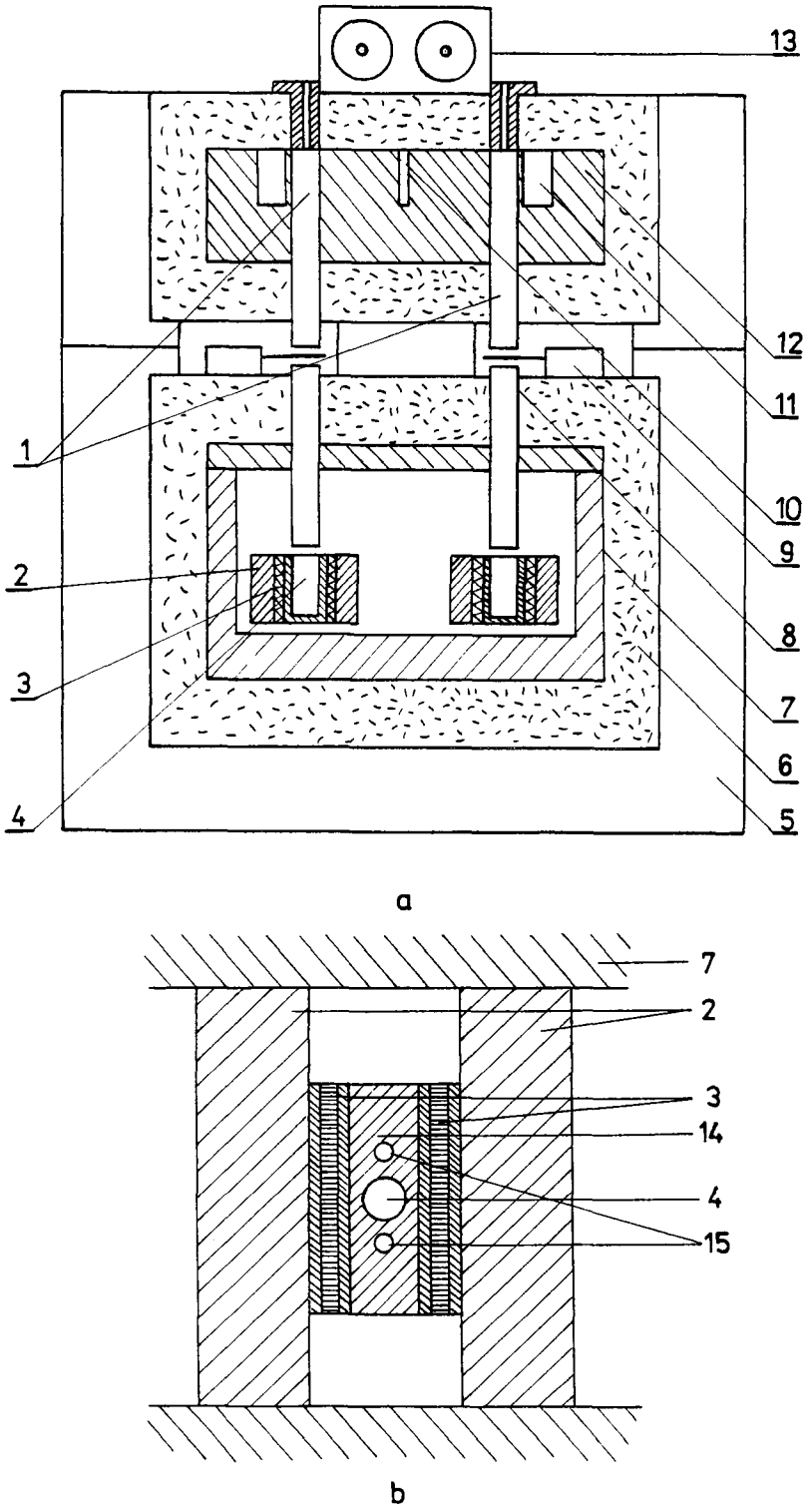


FIG. 10. Drop thermopile-conduction calorimeter for measurements near ambient temperatures (74SUU/WAD)

a. Schematic view of the calorimeter assembly

b. Calorimetric unit seen from above

1—holes for temperature equilibration of the ampoules containing a sample and a reference substance, 2—aluminum block, 3—thermopile plate, 4—receiver, 5—water thermostat, 6—thermal insulation, 7—main heat sink, 8—guiding tube, 9—electromechanical shutter, 10—cavity for temperature controlling element (thermistor), 11—cavity for temperature measuring element (quartz probe), 12—furnace, 13—mechanical lift, 14—aluminum plate, 15—cavities for calibration heaters.

differential signal from the thermopiles is proportional to the difference in the heat capacities of the ampoules. Two experiments are performed; the ampoule dropped on the measuring side of the calorimeter is either empty or filled with a sample and the contents of the ampoule on the reference side remains constant and does not play any role. Using the notation introduced in Eqns. (III-5) and (III-7), the sample heat capacity C is obtained by using the differential thermopile signals A'_{d1} and A'_{d2} corresponding to the first and second experiments, respectively:

$$C = k_c \left(\frac{A'_{d2}}{T_{in2} - T_{rec}} - \frac{A'_{d1}}{T_{in1} - T_{rec}} \right) \qquad \text{(III-12)}$$

where T_{in1} and T_{in2} are the temperatures of the furnace in the two experiments. The calibration constant, k_c, is obtained through electric calibration or measurement with a reference substance of well-known heat capacity. Experiments are fully automated with results accurate to 0.1 percent.

3.2.5. Analysis of Heating and/or Cooling Curves

A variety of techniques was reported in the literature which allow one to calculate heat capacities through the analysis of heating and/or cooling curves. These methods are always comparative and have usually been performed in single-vessel instruments. For instance, the ratio of the heat capacity of the sample C_s and that of a reference substance C_{re} can be obtained by measuring consecutively the rate of temperature change for the two substances:

$$\frac{C_s}{C_{re}} = \frac{(dT_{cv}/d\tau)_{re}}{(dT_{cv}/d\tau)_s}, \qquad \text{(III-13)}$$

where the temperature derivatives are obtained by analyzing heating or cooling curves. Alternatively, the heating times or amounts of heat necessary to produce identical temperature changes in the studied and reference substances are compared. This type of determination was very popular for its simplicity and many values reported between 1920 and 1950 were obtained by this technique. Because of its low accuracy (typically errors of 5 to 10 percent), it is now only used occasionally at high temperatures.

References (33FER/MIL, 41ZIE/MES, 50KUS/CRO) are examples of determinations where the heating times necessary for the identical increase in the temperature of the reference and test substances were measured. Hoffman (52HOF) used constant heating input and maintained a constant gradient between the vessel and its surroundings. A similar principle, with the use of both heating and cooling with a constant temperature gradient, was employed for measurements with liquid sulphur in the temperature range 393-600 K (73KOM/MIL); the instrument is depicted in Fig. 11. Both the quartz cell containing the substance and the reference shield are housed inside a furnace; the difference between these two parts is kept constant during all the experiments. The heat capacity of the substance is obtained by combining the heating times necessary to heat the vessel when it is empty or when filled with sample or when it contains reference substance (copper).

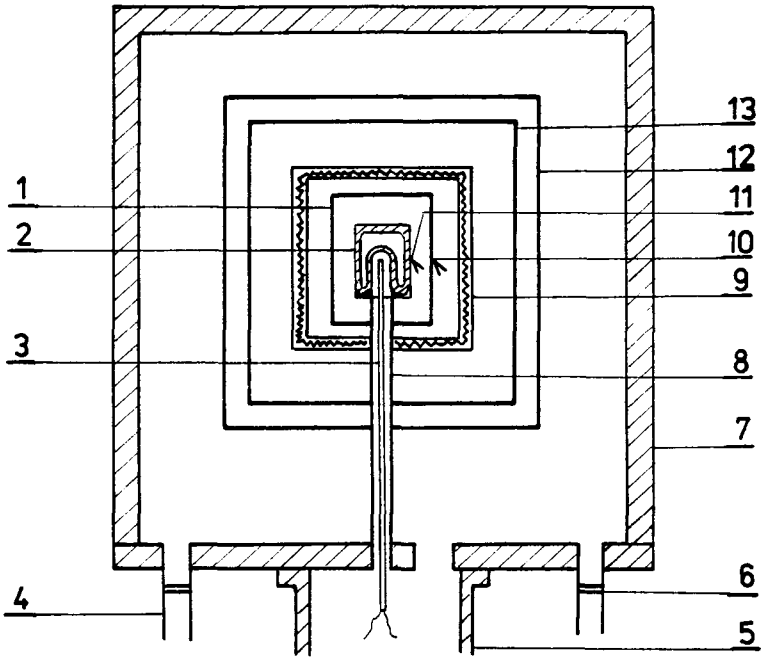


FIG. 11. Constant temperature gradient calorimeter for high temperature measurements (73KOM/MIL)
1—reference jacket, 2—calorimeter vessel (quartz cell inside a metallic shell), 3—thermocouple for measuring temperature, 4—vacuum tight connections for heater leads, 5—vacuum line, 6—vacuum tight connections for thermocouple leads, 7—brass can, 8—supporting tube of quartz, 9—furnace, 10,11—thermocouples for controlling the temperature difference between the reference jacket and calorimeter vessel, 12,13—radiation shield.

3.2.6. Differential Scanning Techniques

As differential scanning techniques, we denote the approaches using the twin vessel arrangement where the temperature of measuring and reference cells are increased simultaneously over a wide temperature range and the effect corresponding to the difference in the thermal response of the two cells is measured directly. These techniques can be performed in commercially available instruments which, in most cases, allow one to work with small samples over a wide temperature range; heating is often continuous but can be also intermittent.

Most instruments work as heat conduction calorimeters in the dynamic mode; the heat is not introduced in some cases (thermopile conduction instruments) into the cell directly but rather into its surroundings. Since the heat capacity of the cells is usually very small compared to that of the surroundings, the T_{cv}, and, T_{su}, are practically identical. Heat leaks from both cells can be considered practically identical and play only a minor role in the heat capacity determination. For a comparison of the thermal response in the two cells, two approaches were developed commercially:

1. *differential thermal analysis* (*DTA*); the temperature difference is measured between the two cells which are heated with identical electrical input energy.
2. *differential scanning calorimetry* (*DSC*); the heating inputs into the measuring and reference cells are adjusted such that the temperature increase in both cells are identical.

DTA and DSC are widely used for investigations with solids (84SES); they are sometimes employed for the measurement of the heat capacities of liquids with an average accuracy of 2 to 5 and 1 to 3 percent, respectively. Examples of the utilization of commercial instruments are the measurements performed on the Dupont 900DTA (67PAC), DTA Mettler TA200 (76ADE/SIM), Dupont 990 DSC (75CUC1), and Perkin-Elmer DSC-2C (87MIL/FEN2) calorimeters.

Mraw and Naas (79MRA/NAA) developed a method for measuring heat capacities of solids using the Perkin-Elmer DSC-2C calorimeter with an error around 1%. This approach was modified by Knipmeyer et al. (89KNI/ARC) in order to allow measurements with liquids up to the vicinity of the critical temperature.

Heat conduction through a thermopile is utilized in several commercial instruments produced by SETARAM. Fig. 12 shows the differential scanning calorimeter DSC111. A thermostatted metallic block can be operated in the temperature range between 150 and 1100 K. The measuring and reference cells are inserted separately into the central parts of two coaxial tubes made of ceramic material (only one is visible in the figure). Thermopiles are housed in the cavities of the metallic block which surround the central parts of the tubes and serve to conduct most of the heat exchanged between the vessel and the surroundings. When the metallic block is heated, the differential signal from the thermopiles reflects the difference in the amounts of heat transferred into the cells, which is proportional to the heat capacity difference between the measuring and reference cells.

A similar principle is used for the measurement of heat capacities of liquids up to 573 K in a modified commercial SETARAM C-80 calorimeter (91COX/QUI). The entire differential assembly is controlled by a computer while the experiments and processing of data are fully automated over the whole operating range of the calorimeter. Typically, the temperature is increased by 10 K steps symmetrical around the temperature plateaus at intervals about 25 K. The procedure consists of three experiments in which the reference vessel is always filled with water and the measuring cell is initially empty, then filled with water, and finally filled with the actual sample. The corresponding differential signals from the thermopiles are denoted as A'_{d1}, A'_{d2}, and A'_{d3}, respectively. As the temperature programming in these three experiments is kept identical, it holds for each temperature increment that:

$$\left[\int_{T_1}^{T_2} c_p \rho \, dT\right]_s = \frac{A'_{d3} - A'_{d1}}{A'_{d2} - A'_{d1}} \left[\int_{T_1}^{T_2} c_p \rho \, dT\right]_{re} \qquad \text{(III-14)}$$

where the terms in brackets on the left- and right-hand sides relate to the sample and reference substance, respectively, and T_1 and T_2 delimit the temperature increment. In this method, ρ and c_p for sample and reference fluids are expressed by polynomials in temperature whose parameters must be known over the whole temperature range of measurement except for the polynomial for the heat capacity of the sample. Its parameters can be obtained after integration by a least squares minimization, thus combining data for all temperature increments. This technique is rapid, yielding isobaric heat capacity directly; the pressure remains constant throughout the measurement as liquid can expand from the vessel. In order to avoid heat leaks in the vertical direction, the calorimeter is operated in an upside down position. The errors are generally below 1 percent. A disadvantage is, however, the necessity to know the density of both the sample and reference fluids over the whole temperature range.

3.2.7. Special Dynamic Methods Using Pulse Heating

Under this title, we group several techniques which use the periodic introduction of heating pulses into the sample and recording of the corresponding temperature oscillations as the principle of measurement. This type of determination is somewhat similar to an analysis of heating or cooling curves described in Section 3.2.5. In most cases, beside heat capacities, the measurements yield thermal conductivities. These techniques are very rapid but lack accuracy (error 2 to 5 percent). They are used most often for very small solid samples and occasionally for liquids usually at extreme conditions (low temperatures, high pressures, experiments in an electromagnetic field). Development of these techniques has been connected with research on superconductors.

Here, we mention briefly only three techniques referenced in Table 4 which summarize the calorimeters; a more detailed overview can be found in several review articles (81LAK/GOP, 82LAK/GOP, 79GME, 87GME). In a *laser-flash method*, a laser beam is used for pulse heating of a sample (79TAK/YOK). Electrical pulses are sent to a heating wire passing through a vessel completely filled with a sample (*hot-wire method*). The same wire serves simulta-

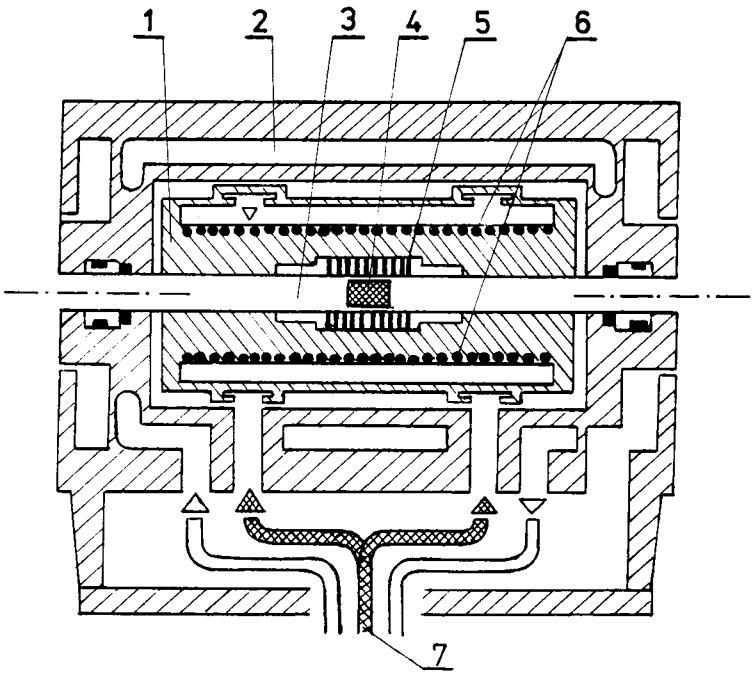


FIG. 12. Scheme of differential scanning calorimeter SETARAM DSC111 (86MER/BEN)
1—metallic bloc, 2—thermostatting unit, 3—one of the two central tubes in ceramics, 4—cell with the sample, 5—thermopile, 6—heating elements, 7—thermostatting system

neously as a temperature element for recording the induced temperature changes (81ATA/ELS). A similar scheme is used in *regular pulsing techniques* (86NAZ/BAS1). A narrow tube with a heating wire at its center passes through the axis of a cylindrical vessel filled with a sample. Periodically either electrical pulses are supplied to the heater or the gaseous cooling agent flows through the tube and temperature oscillations inside the vessel are observed.

3.3. Survey of Calorimeters Used for Determination of Heat Capacities of Pure Liquids

Table 3 divides techniques used for determining heat capacities of pure liquids into groups according to the classification introduced in the preceding sections. The codes defined in Table 2 are used to characterize individual methods and the section numbers refer to the description of the technique in the preceding text.

Table 4 surveys all the calorimeters cited in the original sources of experimental heat capacities which are referenced in this monograph and serve for establishing the data base of raw values. References to instruments with a brief characterization are listed in chronological order in groups defined in Table 3. This division of calorimeters according to the adopted categorization is necessarily a simplification of reality. With respect to the diversity of experimental designs, it is not always possible to associate an instrument unambiguously with a particular group or category.

The terms low, medium, and high are used for indicating the accuracy of measurements with a certain calorimeter in those cases when no quantitative indication was available in the original literature and estimates were made in most cases by the evaluator. For the column *Temperature Range* the meaning is as follows: "low" the lower temperature limit of measurements below room temperature, "medium" 270 - 370 K, "high" the upper temperature limit of measurements above 370 K. For the column *Measurement accuracy* the meaning is as follows: "low" the error is above one percent, "medium" the error is between 0.3 and 1 percent, "high" the error is below 0.3 percent.

4. Previous Compilations of Heat Capacity Data on Liquids

An annotated bibliography is provided which describes the publication of compilations containing reported values for the heat capacities of organic compounds (and some inorganic compounds) from the 19th century through the beginning of 1991. Some compilations provide a thorough coverage of the literature up to about the date of their publication for either organic compounds as an entire class of substances or the coverage may be limited to the gas phase or the condensed phase. These comprise the majority of the compilations listed in this chapter. Other compilations deal with selected classes of organic compounds, such as n-alkanes, 1-alkanols, or organic oxygen compounds, but provide a very detailed evaluation of the experimental data and select optimal heat capacity values for the corresponding class of compounds. Examples of the latter type are: 82WAG/EVA, 85WIL/CHA, 90CHA/GAD, 90ZAB/RUZ, 91RUZ/ZAB and any of the ESDU Series outputs. Some compilations provide a detailed description of the evaluation of the experimental data, such as 70TOU/MAK,

85WIL/CHA, 90ZAB/RUZ, or 91RUZ/ZAB, while others offer only a limited evaluation or quality rating, such as 76TOU/MAK, 84DOM/EVA, or 90DOM/HEA.

Examination of the experimental calorimetric methods from the 19th century to the present reveals improvements not only in experimental techniques resulting in enhanced precision of the data, but shows deliberate and significant attention being directed toward sample purity and sample characterization which assures that the data are also of enhanced accuracy.

Compilations are listed below in chronological order which report data on the heat capacities of liquids. The sustained interest and need for data on heat capacities is exemplified by the growth, continuation, and specificity of these compilations with time.

1897 Berthelot M.P.E., *Thermochimie*, Vol. I and II (*97BER).

Thermochemical (thermodynamic) properties of inorganic and organic compounds are tabulated and the corresponding references are provided whenever possible. The second part of volume II (pp. 393-693) is devoted to the thermochemistry of several hundred organic compounds. Reactions and processes, such as formation, combustion, isomerization, vaporization, fusion, and solution are examined in detail along with the enthalpies for the processes and heat capacities for the various classes of organic compounds (hydrocarbons, alcohols, acids, etc.) in the gas, liquid, solid, and dissolved phases. References are provided with the enthalpy and heat capacity data. This is an excellent summary of 19th century thermochemical research.

1912 *Landolt-Börnstein Physikalisch-Chemische Tabellen*, 4 Auflage, Börnstein R., Roth W.A. (Eds) (12LAN/BOR).

A section on the specific heats of organic compounds (pp. 766-772) lists the heat capacities for about 150 organic compounds in the liquid and solid phases. The data given are compound name, formula, state, temperature or temperature range, specific heat capacity in cal $\cdot$ °C^{-1} $\cdot$ g^{-1} and reference. The precision and accuracy of heat capacity measurements was limited during the 19th century as well as during beginning of the 20th century. Hence, these tables of heat capacity data are more representative of reliable collections of information from the literature but do not appear to be critically evaluated.

1923 *Landolt-Börnstein Physikalisch-Chemische Tabellen*, 5 Auflage, Vol 2., Börnstein R., Roth W.A. (Eds) (23LAN/BOR).

As an up-date from 12LAN/BOR, another section on the specific heat capacities of organic compounds (pp. 1265-1273) lists the values for about 200 organic compounds in the liquid and solid phases. The data provided is similar to that in 12LAN/BOR, also with references.

1927 *Landolt-Börnstein Physikalisch-Chemische Tabellen*, 5 Auflage, Suppl. 1, Börnstein R., Roth W.A. (Eds) (27LAN/BOR).

This collection of heat capacity data on organic substances in the solid and liquid states consists of tables containing about 80 compounds (pp. 692-696) which supplements previous data found in 23LAN/BOR. The supplemental data were extracted from papers published primarily in the 1920's.

1929 *International Critical Tables of Numerical Data, Physics, Chemistry, and Technology*, Vol. V, Washburn E.W. (Ed) (29WAS).

Critically evaluated data on the heat capacities of organic compounds are provided in volume V of the International Critical Tables. Two tables separate organic compounds in the solid state (pp. 101-105, about 125 compounds) from organic compounds in the liquid state (pp. 107-113, about 380 compounds). The data listed are formula, compound name, temperature or temperature range, specific heat capacity in J $\cdot$ °C^{-1} $\cdot$ g^{-1}, percent uncertainty, coefficients in an equation expressing specific heat capacity c_p as a function of temperature, temperature range for the equation, and references.

1931 *Landolt-Börnstein Physikalisch-Chemische Tabellen*, 5 Auflage, Suppl. 2, Vol. II, Roth W.A., Scheel K. (Eds) (31LAN/BOR).

Data on the specific heat capacity, c_p, and heat capacity, C_p, of organic solids and liquids are tabulated (pp. 1194-1217) in a different format with emphasis on providing recent and precise experimental data for specific temperatures and giving a plot of C_p versus temperature for good quality data on about 30 organic compounds. References are primarily to papers published in the 1920's and some during 1930.

1936 *Landolt-Börnstein Physikalisch-Chemische Tabellen*, 5 Auflage, Suppl. 3, Vol. III, Roth W.A., Scheel K. (Eds) (36LAN/BOR).

Data on the specific heat capacity, c_p, and heat capacity, C_p, of organic substances (pp. 2291-2315) are shown as a supplement to the data found in 31LAN/BOR. Experimental data having significant precision are tabulated at specific temperatures, plots of C_p versus temperature are shown for 4 organic compounds as well as a large number of equations representing C_p as a function of temperature.

1950 Timmermans J., *Physicochemical Constants of Pure Organic Compounds*, Vol. I (50TIM).

A thorough search of the chemical literature up to January 1, 1950 was conducted and compiled for physical property data on organic compounds. Particular emphasis was placed upon data for which the purity and characterization of the compounds received attention. Data on the heat capacities of organic compounds was limited to careful measurements for which such data were reported at specified temperatures. Average heat capacity data between two temperatures were rejected.

1952 Rossini F.D., Wagman D.D., Evans W.H., Levine S., Jaffe I., *Selected Values of Chemical Thermodynamic Properties*, National Bureau of Standards, Circular 500 (52ROS/WAG).

Tables of thermodynamic properties of inorganic and one and two carbon atom organic compounds were given after a thorough search, collection, and evaluation of the literature. Tables are divided into Series I and Series II. In Series I, properties listed are heat of formation, free energy of formation, logarithm of the equilibrium constant, entropy, and heat capacity at 298.16 K, and the heat of formation at 0 K. In Series II, phase transition processes, such as fusion, vaporization, sublimation, and solid-solid transitions are described, including the changes in heat, entropy, and heat capacity at the temperature and pressure corresponding to the transition.

1961 *Landolt-Börnstein Physikalisch-Chemische Tabellen*, 6 Auflage, Zahlenwert und Funktionen aus Natur-Wissenschaften und Technik, Vol. II, Part 4, Kalorische Zustandsgrossen (61LAN/BOR).

Separate tables provide data on the thermodynamic properties of organic compounds (pp. 262-372). In these tables, heat capacities are listed for about 550 compounds of which half are in the gas phase. The data provided are formula, compound name, physical state, heat capacity in $J \cdot K^{-1} \cdot mol^{-1}$ at 298 K, and the corresponding reference(s).

1965 Timmermans J., *Physicochemical Constants of Pure Organic Compounds*, Vol. II (65TIM).

Volume II of the Timmermans' compilation is an extension of Volume I (50TIM). The chemical literature is up-dated to 1964. The criteria for choosing physical property data for pure and well-characterized organic compounds is continued. Additional heat capacity data are reported.

1967 Tamplin W.S., Zuzic D.A., *Specific Heat of Organic Hydrocarbons* (67TAM/ZUZ).

After a critical evaluation of the heat capacity data for 83 hydrocarbons, constants are tabulated for an equation of the type: $C_p = A+Bt+Ct^2 \pm D$, where C_p is the heat capacity in $cal \cdot {}^{\circ}C^{-1} \cdot mol^{-1}$, t is the temperature in Celsius, and D is the average difference between the calculated and selected values over the considered temperature range. A total of 84 references are listed.

1968 Wagman D.D., Evans W.E., Parker V.B., Halow I., Bailey S.M., Schumm R.H., *Selected Values of Chemical Thermodynamic Properties*, NBS Technical Note 270-3 (68WAG/EVA).

Selected values were made from the evaluation of available data for the enthalpy and Gibbs function of formation, entropy, and heat capacity at 298.15 K, the enthalpy difference between 298.15 K and 0 K, the enthalpy of formation at 0 K for the first 34 elements and their compounds from the standard order of arrangement. Data for organic compounds were limited to one and two carbon atom compounds. Physical states include crystalline solid, glassy or amorphous solid, liquid, gas, aqueous solution, and some data for non-aqueous solutions. In general, uncertainties are such that they lie between 2 and 20 units of the last figure. No bibliography or commentary are provided. NBS Technical Note 270-3 combines information provided in NBS Technical Notes 270-1 and 270-2, and adds data for two additional elements, zinc and cadmium, and their compounds.

1970 Touloukian Y.S., and Makita T., *Specific Heat of Nonmetallic Liquids and Gases*, Vol. 6 in Thermophysical Properties of Matter (70TOU/MAK).

A careful and critical evaluation is provided for 55 nonmetallic compounds in the gaseous and/or liquid states. References to the reported experimental heat capacity data are given along with information on sample purity and estimated uncertainty in the reported values. A list of recommended C_p values and a polynomial equation for C_p as a function of temperature are also given.

1975 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids. I: Aromatic Hydrocarbons*, Vol. 4 (Item No. 75015) (75ENG).

Heat capacity and enthalpy data for 34 aromatic hydrocarbons have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most

compounds cover the range from the melting temperature to the normal boiling temperature or to the limit of the experimental data whichever is the higher. A total of 36 references is provided.

1975 Horvath A.L., *Physical Properties of Inorganic Compounds* (75HOR).

A critical review was conducted for the physical, thermodynamic, and transport properties of 31 inorganic compounds among which were CO, CO_2, and HCN. Heat capacities are plotted as a function of temperature for the gaseous and condensed phases. Properties at specific temperatures are listed, some of which are: heat of fusion at the melting temperature, heat of vaporization at the boiling temperature, and C_p/C_V for gases at 25 °C. References are provided for each compound listed.

1976 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids. II: Halogenated Methanes*, Vol. 4 (Item No. 76010) (76ENG).

Heat capacity and enthalpy data for 34 halogenated methanes have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most compounds cover the range from the melting temperature to the normal boiling temperature or to the limit of the experimental data whichever is the higher. A total of 24 references is provided.

1976 Miller J.W., Jr., Schorr G.R., Yaws C.L., *Heat Capacities of Liquids* (76MIL/SCH).

Heat capacity data have been correlated for 23 inorganic and 39 organic compounds using a series expansion in temperature of the type: $C_p = A+BT+CT^2+DT^3$, where C_p is the heat capacity of the saturated liquid in cal · K^{-1} · g^{-1} , $A,B,C,D,$ are correlation constants for a specific compound, and T is the temperature in kelvin. In addition to the tabulated correlation constants, the C_p value at 25 °C, the temperature range, and references are given. The correlated data are not recommended for use in the immediate vicinity of the critical temperature, T_c.

1976 Raznjevic K., *Handbook of Thermodynamic Tables and Charts* (76RAZ).

A table is given which lists the specific heats at 20 °C for 22 common solid organic compounds. Another similar table provides specific heats for 82 liquid substances which include organic compounds, inorganic compounds, aqueous solutions, and mixtures. The specific heat data are given, in most cases, at several temperatures. The data do not appear to be evaluated. No references are listed for any property data in this handbook.

1976 Touloukian Y.S. and Makita T., *Specific Heat of Nonmetallic Liquids and Gases*, Suppl. to Vol. 6 in Thermophysical Properties of Matter (76TOU/MAK).

Heat capacities for 210 organic compounds in the gaseous and/or liquid states have been compiled as a by-product publishing 70TOU/MAK. This supplement does not appear to contain the careful and critical evaluation and commentary which was provided in 70TOU/MAK. Tables contain the following: compound name, formula, indication of sample purity, temperature in K, C_p in kJ · K^{-1} · kg^{-1}, pressure, method used, reported accuracy in %, and an internal TPRC accession number. References to original sources for gaseous and liquid heat capacities are frequently not correct. Only about 25% of the references to liquid heat capacity data appear to be satisfactory.

1977 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids. III: Halogenated Ethanes and Ethylenes*, Vol. 4 (Item No. 77007), (77ENG).

Heat capacity and enthalpy data have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most compounds cover the range from the melting temperature to the normal boiling temperature or to the limit of the experimental data whichever is the higher. A total of 42 references is provided.

1979 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids: Aliphatic Alcohols*, Vol. 4 (Item No. 79028) (79ENG).

Heat capacity and enthalpy data for 26 aliphatic alcohols have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most compounds cover the range from the melting temperature, temperature of glass transition, or pour point to a value of the reduced temperature that exceeds 0.5. A total of 42 references is provided.

1979 Herington E.F.G., *Physical Constants of Some Constituents of Coal Tar* (79HER).

Heat capacity data on 80 organic compounds are given at a specified temperature or for a temperature range in J · K^{-1} · g^{-1} . A bibliography and an index of precise C_p measurements which were carried out at NPL are available from another cited NPL Report.

1981 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids: Aliphatic Ketones*, Vol. 4 (Item No. 81030) (81ENG).

Heat capacity and enthalpy data for 20 aliphatic ketones have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most compounds cover the range from the melting temperature to a reduced temperature of about 0.8. A total of 16 references is provided.

1982 Wagman D.D., Evans W.H., Parker V.B., Schumm R.H., Halow I., Bailey S.M., Churney K.L., Nuttall R.L., *The NBS Tables of Chemical Thermodynamic Properties, Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units* (82WAG/EVA).

Reliable values are provided as a result of a thorough evaluation of the available data for the chemical thermodynamic properties of inorganic compounds and organic compounds containing one or two carbon atoms. The properties tabulated are the enthalpy of formation, Gibbs function of formation, entropy, and heat capacity at 298.15 K, the enthalpy difference between 298.15 K and 0 K, and the enthalpy of formation at 0 K. Thermodynamic data for approximately 14 300 substances, in different phases and at different concentrations, are listed. This publication is the combination and culmination of NBS Technical Note 270-1 (October 1965) through NBS Technical Note 270-8 (May 1981). No bibliography or commentary are provided.

1984 Domalski E.S., Evans W.H., Hearing E.D., *Heat Capacities and Entropies of Organic Compounds in the Condensed Phase* (84DOM/EVA).

Heat capacity and entropy data have been compiled for approximately 1400 organic compounds in the liquid and solid phases. Values for the enthalpies and entropies of phase transitions, i.e., solid phase, fusion, vaporization, which were encountered as part of this evaluation, are included. The published literature from about 1925 to 1982 is covered as well as some earlier published papers. The bibliography contains over 850 references. Each referenced article is accompanied by a rating which indicates the quality of the reported data.

1984 Vasil'ev I.A., Petrov V.M., *Thermodynamic Properties of Oxygen-Containing Organic Compounds, Handbook* (84VAS/PET).

Selected thermodynamic properties for 271 organic oxygen compounds have been tabulated from the data available from the literature over the past 60 years. Heat capacity data are among the thermodynamic properties given which have been measured directly or correlated as a function of temperature. The compilation is valuable primarily as a source of data from the Russian literature which are not readily accessible elsewhere. A total of 217 references is listed.

1985 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids: Organic Sulphur Compounds (Thiols and Sulphides)*, Vol. 4 (Item No. 85024) (85ENG).

Heat capacity and enthalpy data for 34 organic sulfur compounds have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most compounds cover the range from the melting temperature to a reduced temperature of 0.86. A total of 24 references is provided.

1985 Wilhoit R.C., Chao J., Hall K.R., *Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. I. Properties of Condensed Phase* (85WIL/CHA).

Data for heat capacities, enthalpies, and phase transitions which have been obtained from calorimetric measurements were examined and critically evaluated on the crystal, glass, and liquid phases for organic oxygen compounds containing one to four carbon atoms per molecule. Equations for the heat capacities expressed as polynomial functions of temperature were fitted to selected data by a least squares procedure. Tables of smoothed values of thermodynamic properties, derived from these functions, are given for 38 organic oxygen compounds. A total of 327 references comprise the bibliography.

1986 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids: Alkanes*, Vol. 4 (Item No. 86007) (86ENG1).

Heat capacity and enthalpy data for 70 alkanes have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and cover the range from the melting temperature to a reduced temperature of 0.96. A total of 80 references is provided.

1986 Engineering Science Data Unit Series, *Heat Capacity and Enthalpy of Liquids: Alkenes and Alkadienes*, Vol. 4 (Item No. 86023) (86ENG2).

Heat capacity and enthalpy data for 34 alkenes and 9 alkadienes have been evaluated and are presented in tabular form as well as in equations as a function of temperature. The data on which the values are based are the most reliable available and for most compounds cover the range from the melting temperature to a reduced temperature of 0.96. A total of 42 references is provided.

1988 Liley P.E., Makita T., Tanaka Y., *Properties of Inorganic and Organic Fluids*, CINDAS Vol. V-1 (88LIL/MAK).

Thermophysical properties, including heat capacities, are given for 10 inorganic and 18 organic fluids as a function of temperature and pressure. Chapters are devoted to individual fluids (i.e., liquid), some of which are: ammonia, chloroform, methane, benzene, sulfur dioxide, methanol, ethanol, water, ethylene glycol, glycerol, toluene, acetylene, and C_5 to C_{10} *n*-alkanes. Data are provided as tables and also in graphical form. An evaluation of the available data is given for each fluid along with the corresponding references. The selected data were used to develop a polynomial expression for the heat capacity of each of the fluids as a function of temperature.

1989 Daubert T.E., Danner R.P., *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, DIPPR® Database*, 4 Volumes (89DAU/DAN).

A compilation containing critically evaluated data on the physical, thermodynamic, and transport properties of over 900 organic compounds has been prepared under the auspices of the Design Institute for Physical Property Research (DIPPR®), which is an AIChE activity. Heat capacity is one of 38 properties of which 13 are, like C_p, temperature dependent. Original or raw experimental data are not provided. Instead, coefficients are given for a specific equation which correlates selected data for a compound whose accuracy has been assessed and identified. An indication is offered as to which data (and references) were used and which were not. The units of C_p in the correlating equations are in $J \cdot K^{-1} \cdot kmol^{-1}$. Specific comments are provided for compounds when necessary. This data compilation is dynamic because it is loose-leaf so that new compounds may be added and data for others may be revised. A bibliography contains 4181 references which covers articles for all 38 properties.

1990 Chao J., Gadella N.A.M., Gammon B.E., Marsh K.N., Rodgers A.S., Somayajulu G.R., Wilhoit R.C., *Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part I. Methanamine, Ethanamine, 1- and 2-Propanamine, Benzenamine, 2-, 3-, and 4-Methylbenzenamine* (90CHA/GAD).

The thermodynamic and thermophysical properties of eight primary amines have been examined and evaluated. Recommended values are given for the following properties: normal boiling temperature, freezing and triple point temperatures, critical constants, thermodynamic properties in the liquid and solid phases, vapor pressure, enthalpy of vaporization, density, second virial coefficients, and enthalpy of combustion. Ideal gas thermodynamic properties were calculated using statistical mechanical procedures. A bibliography contains about 480 references.

1990 Domalski E.S., Hearing E.D., *Heat Capacities and Entropies of Organic Compounds in the Condensed Phase*, Vol. II (90DOM/HEA).

This compilation of data on the heat capacities, entropies, and phase transitions of organic compounds in the condensed phase supplements the work published earlier on this subject (84DOM/EVA). Data on approximately 1300 organic compounds are provided. A total of 565 articles have been examined and evaluated. Each referenced article is provided with a rating which indicates the quality of the reported data. About half of the articles examined contain data published prior to 1982. Most of the 1990 literature is covered.

1990 Zábranský M., Růžička V., Jr., Majer V., *Heat Capacities of Organic Compounds in the Liquid State. I. C_1 to C_{18} 1-Alkanols* (90ZAB/RUZ).

Heat capacities of liquid C_1 to C_{18} 1-alkanols which were determined by calorimetric methods have been compiled and critically evaluated. The selected experimental data were fitted as a function of temperature with cubic splines using weighted least squares minimization. The parameters of the cubic spline polynomials and the recommended values for heat capacities are provided. An assessment of the quality of the recommended data is also given. A new quasi-polynomial equation was derived which permits extrapolation of heat capacities outside of the temperature range of experimental values. The parameters for this equation for C_1 to C_{10} 1-alkanols are presented. Over 140 references are given at the end of the paper. The results of the critical evaluation on C_1 to C_{18} 1-alkanols by 90ZAB/RUZ are part of this compilation.

1991 Marsh K. N. et al., *Selected Values of Thermodynamic Properties of Organic Compounds, TRC Data Project* (91MAR).

Tables of selected values of physical and thermodynamic properties of organic compounds are provided as a function of temperature, separately for hydrocarbons and non-hydrocarbons, in loose-leaf form. The tables are prepared only after an extensive evaluation and correlation of the available data from the literature. This work is a continuation and expansion of 47ROS/PIT and 53ROS/PIT. The expansion has led to an increase in the tabulation of data for the condensed phase over the years. A set of eleven (loose-leaf) volumes constitutes the physical and thermodynamic properties of hydrocarbons while similar information for non-hydrocarbon compounds is found in a set of eight (loose-leaf) volumes. Up-dates to both sets are available twice per year.

1991 Růžička V. Jr., Zábranský M., and Majer V., *Heat Capacities of Organic Compounds in the Liquid State. II. C_1 to C_{18} n-Alkanes* (91RUZ/ZAB).

Heat capacities of liquid C_1 to C_{18} *n*-alkanes which were determined by calorimetric methods have been compiled and critically evaluated. The selected experimental data were fitted as a function of temperature with cubic splines using weighted least squares minimization. The parameters of the cubic spline polynomials and the recommended values for heat capacities are given. Heat capacities were also fitted by a quasi-polynomial equation permitting extrapolation of heat capacities outside of the temperature range of the experimental values. About 150 references are provided at the end of the paper. The results of the critical evaluation on C_1 to C_{18} *n*-alkanes by 91RUZ/ZAB are part of this compilation.

5. Methodology of Data Treatment; Establishment of Recommended Data

5.1. Data Base of Raw Values

Section 1.2. specifies which liquids and what types of heat capacity data (regarding experimental techniques and literature sources) are covered in this compilation. The experimental values extracted from the literature together with auxiliary data were stored in the data base of raw experimental values. This data base covered 1624 substances and consisted of 3389 data sets (set of experimental values from one calorimeter reported by an author for one substance in one original source). Only the parameters for smoothing equations were available for 223 data sets (no discrete data points were reported in these sources). The data sets of discrete values contained 27430 raw data points. The auxiliary data comprised information on the quality of experimental values, sample purity and its determination, the nature of the experimental procedure (calorimetric technique and type of resulting heat capacity) and units used in the original source. This information was used later as a guide in the selection of data sets for the final correlation. Most auxiliary data are summarized for individual substances in tables of experimental heat capacities.

According to the information in the literature sources, we distinguished in the data base of raw values three types of heat capacities: *isobaric heat capacity* C_p, *saturation heat capacity* C_{sat}, and the *average heat capacity* C_{avg}. These three quantities are defined by equations (II-3), (II-4), and (II-18), respectively, and their thermodynamic background is described in Chapter 2.

Below the normal boiling temperature T_{nb} the measured isobaric heat capacity usually relates to atmospheric pressure though this is not frequently specified in the original source. C_p has limited dependence on pressure at low and moderate vapor pressures, and its effect can be neglected unless the pressure change is large. Below the normal boiling temperature no distinction was made between the literature C_p data relating to the saturation line, to atmospheric conditions, or to 101.325 kPa; these were considered as identical. Above the normal boiling temperature, the saturation heat capacities C_{sat} rather than C_p data are reported in the original literature.

Measurements at pressures remote from the vapor pressure are not numerous. They are of interest in studies dealing with mixtures and, hence, no particular attention has been paid to them in the context of this compilation. They were considered only in those cases when they were determined at pressures not far removed from the saturation line or when they extended above the temperature range of the experimental data. They were included only when it was possible to determine with fair accuracy the appropriate correction for their conversion to saturation conditions.

In most calorimetric determinations of heat capacities, the temperature change does not exceed several degrees (temperature steps between 3 and 8 degrees are the most frequent); then, in most cases, the true heat capacity equals the experimental value within the error of measurement. When the temperature change in the experiment is above 10 K, the value obtained is denoted in the following tables as C_{avg}; an exception was made when this type of heat capacity was used for establishing recommended values for several old sources when no other data were available in the corresponding temperature range. In this case Eqn. (II-24) was used for correcting the data to the true heat capacities. Several older data sources (*81VON, *86SCH, *87SCH, 18NAR) were treated in this way and the corresponding deviations in the tables of Correlated Heat Capacities equal zero.

5.2 Evaluation and Selection Process

All available sources were critically assessed. The important part of the selection process was the simultaneous correlation of all experimental data which served to test the consistency and helped to reveal systematic errors. The correlation

was performed by the weighted least-squares method; the *minimized objective function* S had the form:

$$S = \sum_{i=1}^{n} \frac{(C_{sm} - C_{exp})^2}{\sigma^2 C_i} \qquad \text{(V-1)}$$

where the summation is over all the values included in the correlation and the subscript "exp" and "sm" relate to experimental and smoothed values, respectively. The reciprocal of the variance, $\sigma^2 C$, is the *weighting factor*. It was estimated for each value on the basis of the assumed experimental error of the data set used in the correlation. The input information was the percentage error of the experimental data, $\sigma_r C$, as given by the author for the whole data set or estimated by the evaluator in cases where no information was available in the literature. Thus, the variance of the i-th data point was expressed as:

$$\sigma^2 C_i = \left(\frac{C_i \sigma_r C}{100}\right)^2. \qquad \text{(V-2)}$$

The following criteria were observed in the selection process:

1. accuracy of the experimental technique claimed by the author,
2. performance history of the laboratory,
3. consistency of the data with the values from other sources (if available),
4. purity of the substance,
5. type of the calorimeter,
6. time of data origin (measurements published after the year 1940 were preferred),
7. scatter of the data.

It is not, however, possible to apply the above criteria for selecting compounds in a rigorous manner following strictly a certain policy. In many cases, the error of measurement claimed by the author is too optimistic and sometimes does not correspond to reality at all. The evaluating reputation of different laboratories is also a somewhat subjective enterprise. According to our experience the most reliable data were reported from the following laboratories which were preferred in the data selection: BMB, NIPER, NBSW, NBSB, NPLT, and UMAA (the list of acronyms is given in the Section 6.2.1., see below).

Selection and correlation of data for each compound was carried out simultaneously and involved the following steps:

(a) All available heat capacity data sets along with the information on their accuracies were read in and a preliminary joint correlation was performed. If necessary, experimental data were converted to the same type of heat capacity — C_p or C_{sat} (see Section 5.4. for details). Prior to the correlation, data sets considered a priori as unreliable were discarded if more accurate data were available for the same temperature range. However, deviations of the discarded data from the final values were always determined within the temperature range of the recommended values. For those sources where only parameters of a smoothing equation were available, pseudo-discrete data were generated in the temperature range of the parameters' validity. When the number of the experimental data points was not indicated in the original source, a temperature step of 5 to 10 K was used according to the length of the temperature interval and density of data points from other sources.

(b) In the next steps it was possible to make the following tentative changes: to discard individual values, to reject parts of or whole data sets that showed little consistency with the other data, to change weights of whole data sets by altering the expected percent error of measurement, to modify the number of generated pseudo-discrete data points, and to change the temperature limits within which the data sets are considered.

(c) The correlation was repeated several times until the final fit with the selected data was obtained where differences between experimental and smoothed values were roughly equal to or smaller than expected experimental errors. The final correlation of the selected experimental data was assigned a level of accuracy (I to VI, for the definition of levels of accuracy see Section 6.3.3) according to the quality of the correlated data.

The main criterion for judging the quality of the correlation was the *standard weighted deviation*, s_w:

$$s_w = \left(\frac{S_{min}}{n-m}\right)^{1/2}, \qquad \text{(V-3)}$$

where S_{min} is the value of the objective function at its minimum, n is the overall number of the fitted data points, and m is number of independent adjustable parameters in a correlation equation. When experimental data are consistent within the expected error limits, s_w should be close to unity. In addition, use of the following statistical criteria was made:

the *standard deviation*

$$s = \left(\frac{\sum_{i=1}^{n}(C_{sm} - C_{exp})_i^2}{n-m}\right)^{1/2} \qquad \text{(V-4)}$$

the *percentage standard deviation*

$$s_r = \left(\frac{\sum_{i=1}^{n}[(C_{sm} - C_{exp})/C_{exp}]_i^2}{n-m}\right)^{1/2} 100, \qquad \text{(V-5)}$$

the *bias*

$$s_b = \frac{\sum_{i=1}^{n}(C_{sm} - C_{exp})_i}{n}, \qquad \text{(V-6)}$$

and the difference between the number of experimental points with positive and negative deviation from the smoothed values (denoted in tables as +/–).

In order to get information on how data from individual sources compare with the final correlation, the deviations d_w, d, d_r, and d_b defined analogously to s_w, s, s_r and s_b were calculated for both included and rejected data sets. The definitions are as follows:

the *average weighted deviation*

$$d_w = \left(\frac{\sum_{i=1}^{n_1} [(C_{sm} - C_{exp})^2 / \sigma^2 C]_i}{n_1} \right)^{1/2}, \qquad \text{(V-7)}$$

the *average deviation*

$$d = \left(\frac{\sum_{i=1}^{n_1} (C_{sm} - C_{exp})_i^2}{n_1} \right)^{1/2} \qquad \text{(V-8)}$$

the *average percentage deviation*

$$d_r = \left(\frac{\sum_{i=1}^{n_1} [(C_{sm} - C_{exp})/C_{exp}]_i^2}{n_1} \right)^{1/2} 100, \qquad \text{(V-9)}$$

the *bias* of a data set

$$d_b = \frac{\sum_{i=1}^{n_1} (C_{sm} - C_{exp})_i}{n_1}, \qquad \text{(V-10)}$$

where n_1 denotes the number of data points in one data set.

When heat capacity was measured at one temperature only and several literature sources were available, simple selection of the best value or averaging of several measurements was performed.

5.3. Temperature Correlation and Establishment of Recommended Values

Two different approaches were adopted for correlating heat capacities as a function of temperature. *Polynomials* or *cubic spline polynomials* were used for accurately fitting heat capacity inside the temperature limits of experimental values. A *quasi-polynomial equation* was also used when it was appropriate (see below); this equation enabled one to describe the temperature dependence by one set of parameters which, unlike polynomial equations, allows a meaningful extrapolation above the upper temperature limit of the experimental data. Both correlation approaches are described in Section 2.4; here we give only the specifics regarding their use in this project.

5.3.1. Representation of Data by Polynomial(s)

When data are available only in a limited temperature range, one polynomial of third or lower degree may be sufficient for fitting the data successfully. In all cases, when such a condition was probable, the correlation with one polynomial was tried first. Its degree was gradually increased to 3, and the statistical F test was used to determine when the addition of higher terms was not significant any longer.

Fitting with cubic splines was used only when the F test indicated need for a higher than third degree polynomial. We used the correlation algorithm developed at the Technical University of Budapest (79KOL) in which the two boundary conditions are considered during minimization as two additional adjustable parameters. This variant is more flexible than the natural spline. In the first step, three knot temperatures were used (two at the limits and one inside the temperature interval), and if necessary additional knots were added. Usually three and sometimes four knots (i.e. five and six independent parameters, respectively) were necessary for the satisfactory fit of the data within the expected experimental error limits. For exceptional cases, five knots (i.e. seven independent parameters) had to be used for the description of data covering a wide temperature range; in situations where the data sets reached the vicinity of the critical point, the heat capacity increased dramatically.

For many substances, the interior temperature knots were positioned such that the individual subintervals had about the same length. Adjustments were made when the density of experimental points changed significantly with temperature. This was often the case as high-temperature values were usually less numerous than low-temperature measurements. Situations in which one subinterval is almost "empty" are to be avoided. Shorter distances between knot temperatures were also needed when the shape of the heat capacity curve was changing considerably, especially close to the critical point.

The results of spline correlation are usually reported in terms of the knot values and two boundary conditions; the spline routine is then necessary for generating the recommended data. Since such a routine is not available to all users of the data, we preferred to tabulate directly the parameters of the cubic polynomials which are easier to use. This presentation is also consistent with the tabulation when only one polynomial is used. The tabulated adjustable parameters, A_j, relate to the equation expressing the dimensionless quantity C/R as a function of the scaled temperature $T/100$:

$$\frac{C}{R} = \sum_{j=0}^{m} A_{j+1} \left(\frac{T}{100} \right)^j, \qquad \text{(V-11)}$$

where R is the gas constant; scaling was made to improve the numerical stability of the fitting procedure. The upper limit of the summation m is equal to 3 in all cases where the overall temperature range is subdivided (cubic splines fitting) or can be lower when only one polynomial is used to describe the data.

Tables of discrete values were generated using a polynomial representation of the recommended data.

5.3.2. Representation of Data by a Quasi-Polynomial Equation

The quasi-polynomial equation was used in the form:

$$\frac{C}{R} = A_1 \ln(1 - T_r) + \frac{A_2}{1 - T_r} + \sum_{j=0}^{m} A_{j+3} T_r^j, \qquad \text{(V-12)}$$

where $T_r = T/T_c$ and m equals 3 for about 50 % of substances. By combining Eqns. (II-31) and (II-32), it can be shown that the tabulated parameters A_j are constrained as follows: $A_1 = -2(a_2a_3+a_2a_4)$, $A_2 = a_2{}^2$, $A_3 = a_1+2a_2a_4$, $A_4 = a_3{}^2 - 2a_2a_4$, $A_5 = a_3a_4$, $A_6 = a_4{}^2/3$. Parameters a_1, a_2, a_3 and a_4 relate to the Eqn. (II-31) with $m_1 = 1$. For the remaining 50 % of substances Eqn. (V-12) with 4 parameters A_j (m=1) was sufficient. In this case parameters A_5 and A_6 equal zero as a_4 equals zero and the remaining constraints for A_j are modified appropriately.

Under the above conditions, the temperature derivative of the heat capacity is always positive. For some substances, the heat capacity curve has a shallow minimum above the triple point temperature (see Fig.3); in those cases, the nearest experimental temperature above this minimum was selected as the lower limit of the correlation and the data below that temperature were not included. The quasi-polynomial equation was not used when fewer then seven experimental data points were available and the temperature range of experimental data was below 50 K, or when there was no possibility of obtaining the critical temperature.

The variation of heat capacity in the high-temperature range differs considerably from one compound to another. It should be kept in mind that the quasi-polynomial equation is mainly empirical and extrapolation above the upper temperature limit of experimental data is correct only in a qualitative manner. No guarantee can be given that the extrapolation will describe quantitatively the real heat capacity in this region except for the value at the critical point which is always correct and corresponds to plus infinity.

For organic substances, the critical temperatures from the data bank of the Prague Institute of Chemical Technology (91CDA) or from the TRC tables (91MAR) were used; for substances where T_c values were not found, estimates were performed according to Lydersen (55LYD). The compilation by Morachevskii and Sladkov (87MOR/SLA) was used as the main source of critical temperatures for inorganic substances.

The following expressions were derived for the calculation of the enthalpy and entropy differences when using the quasi-polynomial equation:

$$\frac{\Delta H}{RT_c} = A_1[(T_{r2}-1)\ln(1-T_{r2}) - (T_{r1}-1)\ln(1-T_{r1}) - (T_{r2}-T_{r1})]$$

$$- A_2[\ln(1-T_{r2}) - \ln(1-T_{r1})] + A_3(T_{r2}-T_{r1}) \qquad \text{(V-13)}$$

$$+ \frac{A_4}{2}(T_{r2}^2 - T_{r1}^2) + \frac{A_5}{3}(T_{r2}^3 - T_{r1}^3) + \frac{A_6}{4}(T_{r2}^4 - T_{r1}^4)$$

$$\frac{\Delta S}{R} = A_1[\text{dilog}(1-T_{r1}) - \text{dilog}(1-T_{r2})]$$

$$+ A_2[\ln(T_{r2}) - \ln(1-T_{r2}) - \ln(T_{r1}) + \ln(1-T_{r1})] \qquad \text{(V-14)}$$

$$+ A_3(\ln T_{r2} - \ln T_{Nr1}) + A_4(T_{r2} - T_{r1})$$

$$+ \frac{A_5}{2}(T_{r2}^2 - T_{r1}^2) + \frac{A_6}{3}(T_{r2}^3 - T_{r1}^3)$$

where dilog (x) can be approximated by the following function

$$\text{dilog}(x) = \frac{D_1+D_2x+D_3(x-0.1)^2+D_4(x-0.1)^3+D_5(x-0.1)^4+D_6(x-0.1)^5}{D_7+D_8x+D_9(x-0.1)^2+D_{10}(x-0.1)^3+D_{11}(x-0.1)^4+D_{12}(x-0.1)^5} \qquad \text{(V-15)}$$

where

D_1 =	−1.168876770,	D_2 =	24.68591493,
D_3 =	145.8845448,	D_4 =	242.8099791,
D_5 =	−178.5653452,	D_6 =	−338.8035369,
D_7 =	−1.096178670,	D_8 =	20.96178670,
D_9 =	150.3249552,	D_{10} =	427.9410776,
D_{11} =	414.7775590,	D_{12} =	69.55852420.

5.4. Types of Heat Capacities Presented

When establishing the recommended values no distinction was made between the saturation heat capacity C_{sat} and the isobaric heat capacity C_p when their difference was smaller than the expected error of experimental data over the whole temperature range of their validity. This was the case for practically all substances where data did not reach above the normal boiling temperature. Then only one set of parameters was presented for each of the correlation equations and only one set of discrete values was generated.

For the compounds where experimental values of reasonable accuracy are available above the normal boiling temperature, distinct recommended data sets are presented for C_p and C_{sat}. In this case, all raw data were first converted to one type of heat capacity which was used in the evaluation and selection process. After the experimental values for the final correlation had been set, they were expressed as C_p and C_{sat} and both sets were correlated separately under identical conditions using the polynomial or cubic spline representation. Only isobaric heat capacity C_p was correlated by the quasi-polynomial equation.

Recommended C_{sat} data relate by definition to the saturation line. Recommended C_p data relate above the normal boiling temperature to the saturation line. Below T_{nb}, they represent both the heat capacity at standard pressure 101.325 kPa and the saturation pressure as their difference is smaller then the accuracy of the best literature data.

Thermodynamic relationships between isobaric and saturation heat capacities are discussed in detail in Section 2.1. When necessary, conversion between C_p and C_{sat} was performed using Eqn. (II-6). As there are not enough data

on expansivities, the term $(\partial V/\partial T)_p$ was approximated by $(\partial V/\partial T)_{sat}$; the difference between them becomes important only far above the normal boiling temperature. The latter term was calculated from the temperature correlation of densities along the saturation line using a modified Rackett equation (85CAM/THO) or the Francis equation (86SMI/SRI). The derivative $(dp/dT)_{sat}$ was calculated from one of the following vapor pressure equations: Wagner, Frost-Kalkwarf, Cox or Antoine using parameters from the references 83MCG, 79DYK/REP, 90CHI/GAM, 92STE/CHI2 respectively. More specific information regarding individual substances is given when appropriate in the introductory discussions before the tables.

5.5. The Influence of Changes in Atomic Masses on the Heat Capacity Value

The values of atomic masses of elements are being continuously refined. When converting the primary measured data to the heat capacities the individual authors were using molar masses valid at the time of experiment. Thus the later modifications of molar masses necessarily also affect the heat capacity values; logically the most influenced are the old measurements. We have analyzed and evaluated the effect of the change in atomic masses on the heat capacity for three compounds, n-heptane, ethanol, and triethylamineborane, for which accurate raw data are available. The results of the evaluation are given in Table 5. The systematic error in the heat capacity due to the change in molar mass is equal to the percent difference in the original and the reference molar masses. It is apparent from the table that this error is at least one order of magnitude smaller when compared to the error in the data. The atomic masses recommended by the IUPAC Commission on Atomic Weights and Isotopic Abundances (91COM) were used as reference values throughout the publication.

TABLE 5. Examples of the systematic error Δ in the heat capacities measured over the last 60 years due to the change in atomic masses of elements.

Data source	Year	σ_r[a]/%	Molar mass	Δ[b]/%
		n-heptane		
47OSB/GIN	1947	0.1	100.198	6.10^{-3}
54DOU/FUR	1954	0.1	100.205	-1.10^{-3}
61HUF/GRO	1961	0.2	100.20557	-2.10^{-3}
79SCH/OFF	1979	0.1	100.2034	-6.10^{-4}
		ethanol		
31FIO/GIN	1931	0.2	46.0468	5.10^{-2}
68PAZ/REC	1968	0.1	46.0694	-8.10^{-4}
76FOR/BEN1	1976	0.3	46.0688	5.10^{-4}
79BRO/ZIE	1979	0.2	46.0688	5.10^{-4}
		triethylamineborane		
67SMI/GOO1	1967	0.2	115.0267	-7.10^{-5}
70FIN/TOD	1970	0.2	115.0249	1.10^{-3}

[a] measurement error of the original data

[b] $\Delta = 100 \cdot (\text{molar mass}_{1991} - \text{molar mass}_{year}) / \text{molar mass}_{1991}$

5.6. Conversion of Temperatures and Original Heat Capacity Data to the International Temperature Scale of 1990

Most experimental data which served for producing the recommended data in this compilation were published over the last 60 years. During this period three different temperature scales (ITS-27, IPTS-48 and IPTS-68) were in use. Since the beginning of 1990, ITS-90 has been the standard. We have closely examined the effect which the introduction of the new temperature scale has to the published heat capacity values. Main points are as follows.

a. *What are the differences between the different temperature scales?*

Table 6 lists the differences between ITS-90 and the previous two temperature scales in the temperature range between −180 and 300 °C where most data compiled here were reported (data at higher temperatures are always subject to errors which are much larger than any changes due to a scale conversion). ITS-48 is identical with ITS-27 below 630 K. Temperature derivatives of the differences are also listed; they play a more important role in conversion than the shifts in temperature (see below). Note that starting with 473 K the differences between IPTS-68 and IPTS-48 are greater than between ITS-90 and the previous two scales (see Table 6).

b. *How to correct heat capacities for a change in the temperature scale*

When converting heat capacity values to ITS-90 two effects have to be considered.

Firstly, the temperatures, to which the experimental heat capacities are related, have to be converted. This procedure is trivial and has little effect upon the heat capacity except in the region close to the critical point where the variation with temperature is steep. In other cases, the correction in the heat capacity due to temperature shift rarely exceeds 0.02 percent and is typically one order of magnitude lower.

Secondly, the heat capacities are usually determined as a ratio of energy to the corresponding temperature increment ΔT. This increment can be affected by the scale change in a more substantial manner than T itself, especially at temperatures where $d((\delta T)/dT)$ has a large value (see Table 6); the changes in ΔT are typically several hundredths of a percent and attain in the most unfavorable cases as much as 0.09 and 0.03 percent for conversion from IPTS-48 and IPTS-68, respectively, for the compounds and temperature ranges considered herein. The percent change in the heat capacity is then identical.

It is clear that both effects are interrelated and can add to or compensate for each other depending on the shape of the δT versus T function. Specific examples in Tables 7 to 12 demonstrate the effects of conversion from IPTS-48 and IPTS-68 for the heat capacities of organic compounds for a wide temperature range.

c. *Is conversion of heat capacities C_{sat} and C_p to ITS-90 feasible?*

For converting the data to ITS-90 scale, it is necessary to have the following information:

— temperature scale used; this information is not often given explicitly in the original literature but can be guessed from the year of publication

— temperature increments for individual data points; this information is unfortunately missing in most data sources. It is systematically given only in the articles from the former National Bureau of Standards, Washington D.C. (now called NIST) for a very limited number of compounds and for a part of data reported by the former National Bureau of Mines, Bartlesville, Oklahoma (now called NIPER). For extending the temperature range of recommended values, the above sources are often combined with other data for which conversion is not possible. A partial conversion of data serving to produce the recommended values would mean the introduction of certain inconsistencies.

TABLE 6. Approximate differences $\delta = (t_{90} - t_{48})/°C$ and $\delta = (t_{90} - t_{68})/°C$ and derivatives of these differences (based on values reported by 92GOL/WEI)

IPTS-48			IPTS-68		
$t_{48}/°C$	δ	$(d\delta/dT) \cdot 10^5$	$t_{68}/°C$	δ	$(d\delta/dT) \cdot 10^5$
−180	0.020	00	−180	0.008	20
−170	0.017	−46	−170	0.010	20
−160	0.007	−82	−160	0.012	13
−150	0.000	00	−150	0.013	10
−140	0.001	18	−140	0.014	00
−130	0.008	79	−130	0.014	00
−120	0.017	90	−120	0.014	00
−110	0.026	90	−110	0.013	00
−100	0.035	72	−100	0.013	00
−90	0.041	48	−90	0.012	00
−80	0.045	00	−80	0.012	00
−70	0.045	00	−70	0.011	−10
−60	0.042	−34	−60	0.010	−10
−50	0.038	−48	−50	0.009	−10
−40	0.032	−69	−40	0.008	−13
−30	0.024	−80	−30	0.006	−20
−20	0.016	−80	−20	0.004	−20
−10	0.008	−80	−10	0.002	−20
0	0.0	−69	0	0.0	−20
10	−0.006	−60	10	−0.002	−24
20	−0.012	−48	20	−0.005	−24
30	−0.016	−40	30	−0.007	−24
40	−0.020	−34	40	−0.010	−30
50	−0.023	−30	50	−0.013	−30
60	−0.026	00	60	−0.016	−24
70	−0.026	00	70	−0.018	−24
80	−0.027	00	80	−0.021	−30
90	−0.027	00	90	−0.024	−24
100	−0.026	13	100	−0.026	−20
110	−0.024	13	110	−0.028	−20
120	−0.023	15	120	−0.030	−20
130	−0.020	24	130	−0.032	−20
140	−0.018	20	140	−0.034	−20
150	−0.016	27	150	−0.036	−13
160	−0.012	34	160	−0.037	−10
170	−0.009	34	170	−0.038	−10
180	−0.005	40	180	−0.039	00
190	−0.001	40	190	−0.039	00
200	0.003	40	200	−0.040	00
210	0.007	40	210	−0.040	00
220	0.011	34	220	−0.040	00
230	0.014	34	230	−0.040	00
240	0.018	34	240	−0.040	00
250	0.021	30	250	−0.040	00
260	0.024	34	260	−0.040	00
270	0.028	27	270	−0.039	00
280	0.030	20	280	−0.039	00
290	0.032	20	290	−0.039	00
300	0.034	13	300	−0.039	00

Heat capacities and the corresponding temperatures published in the literature cannot always be considered strictly as raw values. The results of measurements are in some cases "smoothed" graphically or with a computer program before tabulation (listed temperatures are very often rounded values). There is usually little information on such data treatment in original data sources; it can be, however, assumed that during smoothing the heat capacity is already subject to shifts comparable or even larger than those corresponding to the scale changes; hence, real "raw values" are frequently not available. In these cases, adjustments in the heat capacities due to any temperature scale changes become highly questionable (see Tables 7 to 12 for examples) and application of the conversion formula by Douglas (69DOU) as presented by Goldberg and Weir (92GOL/WEI) is not possible.

It is obvious from the above considerations that conversion of heat capacities to the basis of ITS-90 is not always a straightforward process since the needed information is often missing. Also, since the changes in the heat capacities that would be produced are almost always less than the accuracy of the heat capacities, the conversion is very rarely called for.

d. *Magnitude of the changes in the heat capacity and in the uncertainty of recommended data*

The reliability of recommended data is expressed in this monograph by six uncertainty classes. The best uncertainty class I (error below 0.1 percent) is used only for three compounds (*n*-heptane, ethanol, benzothiazole) in a part of the temperature interval where experimental data measured by different authors were reported. The next class II (error below 0.3 percent) covers about 200 compounds. Considering the magnitude of changes in C_p due to the temperature scale shifts, it seems reasonable to correct only the data for "class I compounds". For the above three compounds with the class I uncertainty, the necessary auxiliary information required for conversion to ITS-90 is available only for two compounds: n-heptane (three data sets, see Table 13) and for ethanol (one data set 77HAI/SUG).

e. *Conclusions regarding temperature scale changes*

Upon consideration of the factors given above, the conversion of experimental data to ITS-90 turned out to be either questionable or unnecessary.

The following six tables illustrate the effect of temperature scale changes on heat capacities using as examples four compounds measured at the former Bureau of Mines at Bartlesville, Oklahoma; temperature increments were always available in the original literature. Tables 7 to 9 illustrate conversion from IPTS-48 to ITS-90, Tables 10 to 12 are examples of conversion from IPTS-68 to ITS-90. Temperature in the first column corresponds to IPTS-48 or IPTS-68 in the relationship to the heat capacities in the second column and to ITS-90 in the relationship to the third column. Differences (in percent) are listed in the last column of all tables.

Two different ways in converting the data are demonstrated:

1. In Tables 7,8,10 and 11 the temperatures and heat capacities reported in the original source were converted to ITS-90 (both the effects on T and ΔT were taken into consideration). Subsequently both original and converted data were

smoothed separately by third degree polynomials which served for generating the values at the listed rounded temperatures.

2. In Tables 9 and 12 the temperatures and heat capacities reported in the original source were converted to ITS-90 in the same way as under 1. Subsequently only the converted data were smoothed by a third degree polynomial which served for generating ITS-90 heat capacity values at the temperatures identical to those given in the original source.

Comparison of percent differences for the cases where heat capacities for an identical compound were treated differently (Tables 8 and 9 and Tables 11 and 12) shows that both approaches to the conversion give comparable results.

Examination of the magnitude of differences in heat capacities due to the temperature scale change reveals that they are at least two times smaller that the measurement error.

TABLE 7. Conversion of saturation heat capacities from IPTS-48 to ITS-90 for 2,2-dimethylpentane (61HUF/GRO, measurement precision and measurement accuracy 0.1 % and 0.2 %, respectively). Comparison of smoothed data.

T K	C_{48} J · K^{-1} · mol^{-1}	C_{90} J · K^{-1} · mol^{-1}	$100 \cdot (C_{48}-C_{90})/C_{90}$ %
160	167.07	166.91	0.10
170	170.12	169.99	0.08
180	173.33	173.22	0.06
190	176.68	176.61	0.04
200	180.16	180.14	0.01
210	183.79	183.81	–0.01
220	187.55	187.62	–0.04
230	191.45	191.55	–0.05
240	195.47	195.60	–0.07
250	199.61	199.77	–0.08
260	203.88	204.05	–0.08
270	208.26	208.43	–0.08
280	212.76	212.91	–0.07
290	217.36	217.48	–0.06
300	222.08	222.14	–0.03

TABLE 8. Conversion of saturation heat capacities from IPTS-48 to ITS-90 for 1-(ethylthio)propane (61MCC/FIN, measurement precision and measurement accuracy 0.1 % and 0.2 %, respectively). Comparison of smoothed data.

T K	C_{48} J · K^{-1} · mol^{-1}	C_{90} J · K^{-1} · mol^{-1}	$100 \cdot (C_{48}-C_{90})/C_{90}$ %
160	180.63	180.39	0.13
170	180.36	180.20	0.09
180	180.40	180.31	0.05
190	180.74	180.70	0.02
200	181.35	181.36	–0.01
210	182.22	182.27	–0.03
220	183.33	183.41	–0.04
230	184.66	184.77	–0.06
240	186.20	186.32	–0.06
250	187.93	188.06	–0.07
260	189.84	189.97	–0.07
270	191.89	192.03	–0.07
280	194.09	194.22	–0.07
290	196.41	196.53	–0.06
300	198.83	198.94	–0.06
310	201.34	201.43	–0.04
320	203.92	203.99	–0.03
330	206.56	206.61	–0.02
340	209.22	209.26	–0.02
350	211.91	211.93	–0.01
360	214.60	214.60	0.00
370	217.27	217.25	0.01

TABLE 9. Conversion of saturation heat capacities from IPTS-48 to ITS-90 for 1-(ethylthio)propane (61MCC/FIN, measurement precision and measurement accuracy 0.1 % and 0.2 %, respectively). Comparison of the smoothed data (ITS-90) with the raw values reported in the literature source (IPTS-48).

T K	C_{48} J · K^{-1} · mol^{-1}	C_{90} J · K^{-1} · mol^{-1}	$100 \cdot (C_{48}-C_{90})/C_{90}$ %
165.59	180.44	180.25	0.11
171.78	180.35	180.20	0.08
181.88	180.45	180.37	0.04
197.08	181.15	181.15	0.00
217.30	183.01	183.08	–0.04
237.22	185.76	185.87	–0.06
257.28	189.30	189.44	–0.07
278.36	193.73	193.85	–0.06
288.71	196.11	196.22	–0.06
298.39	198.44	198.54	–0.05
308.40	200.94	201.03	–0.04
328.08	206.05	206.10	–0.02
347.24	211.17	211.19	–0.01
356.67	213.71	213.71	0.00
366.02	216.22	216.20	0.01

TABLE 10. Conversion from IPTS-68 to ITS-90 for 1-methylpyrrole (88MES/TOD, measurement precision and measurement accuracy 0.05 % and 0.1 %, respectively). Comparison of smoothed data.

T K	C_{68} J · K^{-1} · mol^{-1}	C_{90} J · K^{-1} · mol^{-1}	$100 \cdot (C_{68}-C_{90})/C_{90}$ %
230	137.64	137.66	–0.01
240	139.03	139.05	–0.01
250	140.61	140.64	–0.02
260	142.35	142.38	–0.02
270	144.23	144.27	–0.03
280	146.22	146.26	–0.03
290	148.30	148.34	–0.03
300	150.46	150.50	–0.03
310	152.69	152.73	–0.03
320	154.97	155.02	–0.03
330	157.31	157.36	–0.03
340	159.69	159.73	–0.03
350	162.09	162.14	–0.03
360	164.52	164.56	–0.02

TABLE 11. Conversion from IPTS-68 to ITS-90 for (Z)-2-hexene (90MES/TOD, measurement precision and measurement accuracy 0.05 % and 0.1 %, respectively). Comparison of smoothed data.

T K	C_{68} J · K^{-1} · mol^{-1}	C_{90} J · K^{-1} · mol^{-1}	$100 \cdot (C_{68}-C_{90})/C_{90}$ %
130	154.07	154.06	0.01
140	153.39	153.38	0.01
150	153.03	153.03	0.00
160	152.98	152.98	0.00
170	153.24	153.24	0.00
180	153.78	153.78	0.00
190	154.60	154.61	–0.01
200	155.69	155.70	–0.01
210	157.03	157.05	–0.01
220	158.62	158.64	–0.01
230	160.44	160.47	–0.02
240	162.49	162.52	–0.02
250	164.75	164.78	–0.02
260	167.21	167.25	–0.02
270	169.86	169.90	–0.02
280	172.69	172.73	–0.02
290	175.69	175.74	–0.03
300	178.85	178.90	–0.03
310	182.15	182.20	–0.03
320	185.59	185.64	–0.03

TABLE 12. Conversion from IPTS-68 to ITS-90 for (Z)-2-hexene (90MES/TOD, measurement precision and measurement accuracy 0.05 % and 0.1 %, respectively). Comparison of the smoothed data (ITS-90) with the raw values reported in the literature source (IPTS-68).

T K	C_{68} J · K^{-1} · mol^{-1}	C_{90} J · K^{-1} · mol^{-1}	$100 \cdot (C_{68}-C_{90})/C_{90}$ %
129.062	154.15	154.14	0.01
137.174	153.55	153.54	0.01
162.026	153.01	153.01	0.00
180.930	153.85	153.85	0.00
200.557	155.76	155.77	–0.01
221.615	158.90	158.92	–0.01
242.141	162.96	162.99	–0.02
263.156	168.03	168.07	–0.02
284.157	173.92	173.96	–0.02
300.630	179.05	179.10	–0.03
314.445	183.66	183.72	–0.03

The only compound where the conversion was performed was n-heptane which is used as the primary calorimetric standard for heat capacity measurements of liquids. Accurate raw experimental data measured at the National Bureau of Standards (NBS), Washington D.C. (47OSB/GIN, 54DOU/FUR) and at the Bureau of Mines (BM), Bartlesville, Oklahoma (61MCC/MES) have been critically selected from all available sources and converted to ITS-90. The conversion procedure was rather complex and was described in 94ZAB/RUZ. Heat capacities converted to ITS-90 and differences between the original heat capacities that relate to IPTS-48 and those converted to ITS-90 are presented in Table 13. Both IPTS-48 and ITS-90 values were generated from a smoothing equation. Differences in heat capacities due to the conversion to ITS-90 are of the same magnitude as the measurement error of the NBS and the BM data. A joint correlation of converted data from the two laboratories provided recommended heat capacities of n-heptane that are given in the last column of Table 13.

Our recommendations differ to some extent from those published for n-heptane in the IUPAC publication on reference materials (88MAR). The previous recommendations are based exclusively on the NBS data (54DOU/FUR). The evaluators (A.J. Head and R. Sabbah) converted temperatures to IPTS-68; however no corrections were applied to the experimental heat capacities, although it was possible to do so by using information in the original paper. In producing our recommendations, we were converting both temperatures and heat capacity values to ITS-90 and also made a correction using the latest values of molecular masses.

TABLE 13. Heat capacity of n-heptane converted to ITS-90.

	NBS data		BM data		Recommended values
T_{90} K	C_{sat} J · K^{-1} · mol^{-1}	d[a] %	C_{sat} J · K^{-1} · mol^{-1}	d[a] %	C_{sat} J · K^{-1} · mol^{-1}
182.603	202.84[b]	0.15	202.77[b]	0.12	202.80[b]
190	201.79	0.08	201.89	0.03	201.84
200	201.32	–0.01	201.50	–0.02	201.38
210	201.67	0.01	201.90	–0.05	201.74
220	202.74	0.00	202.97	–0.04	202.81
230	204.41	–0.02	204.62	–0.05	204.48
240	206.60	–0.06	206.75	–0.07	206.66
250	209.18	–0.01	209.28	–0.08	209.24

TABLE 13. Heat capacity of n-heptane converted to ITS-90—(Continued)

	NBS data		BM data		Recommended values
T_{90} K	C_{sat} J · K^{-1} · mol^{-1}	d[a] %	C_{sat} J · K^{-1} · mol^{-1}	d[a] %	C_{sat} J · K^{-1} · mol^{-1}
260	212.07	–0.16	212.14	–0.08	212.12
270	215.17	–0.17	215.26	–0.11	215.21
280	218.45	–0.10	218.59	–0.11	218.48
290	221.92	–0.08	222.10	–0.08	221.94
298.15	224.88[c]	–0.06	225.08	–0.07	224.88
300	225.56	–0.05	225.76	–0.05	225.57
310	229.38	–0.05	229.55	–0.03	229.37
320	233.35	–0.04	233.47	–0.04	233.33
330	237.48	–0.04	237.50	–0.03	237.45
340	241.76	–0.04	241.69	–0.01	241.72
350	246.18	–0.04	246.04	–0.02	246.14
360[d]	250.74	–0.04	250.60	–0.01	250.69
370	255.43	–0.05	255.41[b]	–0.01	255.37
380	260.24	–0.05			260.18
390	265.16	–0.05			265.10
400[e]	270.19	–0.02			270.14
410	275.33	0.01			275.30
420	280.62	0.05			280.61
430	286.11	0.07			286.11
440	291.84	0.06			291.85
450	297.86	0.03			297.88
460	304.21	–0.02			304.24
470	310.94	–0.09			310.98
480	318.11	–0.12			318.13
490	325.74	0.00			325.75
500	334.91	0.22			334.89
510	350.69	–0.13			350.66
520	379.15	0.06			379.16

[a] $d = (C_{48} - C_{90}) \cdot 100/C_{90}$, heat capacities calculated at the same numerical value of temperature in IPTS–48 and in ITS–90

[b] extrapolated

[c] temperature in the original source 54DOU/FUR is 298.16 K

[d] data from NBS above this temperature were derived from enthalpy measurements by drop calorimetry; their accuracy is substantially lower compared to adiabatic measurements below this temperature. Only the temperature shift was considered at $T > 360$ K (no ΔT correction)

[e] n–heptane is not a calorimetric standard above this temperature

5.7. Units and Conversion Factors

All numerical data reported in the tables are given in SI units. Factors for converting the values from the original sources to SI units are as follows:

1 cal_{th} = 4.1840 J
1 cal_{IT} = 4.1868 J
1 Btu_{th} $lb^{-1}(°F)^{-1}$ = 4.1840 J · K^{-1} · g^{-1}
1 Btu_{IT} $lb^{-1}(°F)^{-1}$ = 4.1868 J · K^{-1} · g^{-1}
T/K = t/°C + 273.15
T/K = T/°F · 0.55555 + 255.37
R = 8.31451 J · K^{-1} · mol^{-1}

where subscript "th" and "IT" denote the thermochemical basis and the International Steam Tables basis, respectively. In many cases, it is not clear which basis was used in the original source; for data in calories it was usually the thermochemical basis and for those in $Btu_{IT}lb^{-1}(°F)^{-1}$ the IT basis. During the course of this project the recommended value of the universal gas constant R was modified by the CODATA Fundamental Constants Task Group (88COH/TAY) from 8.31441 to 8.31451 J · K^{-1} · mol^{-1}; the latter value was used throughout this compilation.

6. Guide to Tables

6.1. Division of Substances into Groups

To make the data presentation logical and easy to follow, the compounds are divided into *sections* according to the kinds of atoms they contain. These are further divided into *groups* according to their chemical structure. This arrangement makes it possible to illustrate specific features of individual families of substances and to show the connection between the magnitude of the quantities listed and the chemical structure of individual substances. The adopted ordering system can be seen in the following table. Each group is assigned a designated double digit.

Table 14. Division of Compounds into Groups

0. Inorganic substances
   - 01. Elements
   - 02. Inorganic compounds

1. Compounds of Carbon and Hydrogen
   - 11. Saturated aliphatic hydrocarbons
   - 12. Saturated cyclic hydrocarbons
   - 13. Unsaturated aliphatic hydrocarbons
   - 14. Aromatic and unsaturated cyclic hydrocarbons

2. Compounds of Carbon, Hydrogen and Halogen
   - 21. Fluorine derivatives
   - 22. Chlorine derivatives
   - 23. Bromine derivatives
   - 24. Iodine derivatives
   - 25. Mixed halogen derivatives

3. Compounds of Carbon, Hydrogen and Nitrogen
   - 31. Amines
   - 32. Nitriles
   - 33. Heterocyclic nitrogen compounds
   - 34. Miscellaneous nitrogen compounds

4. Compounds of Carbon, Hydrogen and Oxygen
   - 41. Ethers
   - 42. Alcohols and phenols
   - 43. Carbonyl compounds
   - 44. Acids and anhydrides
   - 45. Esters
   - 46. Heterocyclic oxygen compounds
   - 47. Miscellaneous oxygen compounds

5. Compounds of Carbon, Hydrogen and Sulfur
   - 51. Sulfides
   - 52. Thiols
   - 53. Heterocyclic sulfur compounds

6. Other Organic Compounds Containing Halogens, Nitrogen, Oxygen and Sulfur
   - 61. Compounds of carbon, hydrogen, halogen and oxygen
   - 62. Compounds of carbon, hydrogen, nitrogen and oxygen
   - 63. Compounds of carbon, hydrogen, oxygen and sulfur
   - 64. Miscellaneous compounds

7. Organic Compounds Containing Other Elements than Halogens, Nitrogen, Oxygen and Sulfur
   - 71. Organosilicon compounds
   - 72. Organic compounds containing phosphorus and boron
   - 73. Organometallic compounds
   - 74. Salts of organic acids

The substances of section 0 (elements and inorganic compounds) are ordered according to their formulas in alphabetical order. Organic compounds (sections 1 to 7) are ordered within each group according to the usual convention (Hill system); i.e., in order of increasing number of carbon and hydrogen atoms. Other elements are placed in alphabetical order. The substances having the same molecular formula are arranged in alphabetical order according to their names. Each substance is coded by two numbers separated by a dash. The first two-digit number indicates the group (family of substances), and the second three-digit number denotes the serial number of a substance inside the group. In naming the substances, we adopted the Chemical Abstracts rules for the names under which the substance was presented with exception of simple esters where we used shorter names, e.g., methyl acetate instead of methyl ester acetic acid. Codes for individual substances permitting their location inside the tables and the corresponding CAS registry numbers can be found in the formula and name indices at the end of the compilation.

6.2. Introductory Texts for Individual Groups

A short introduction precedes the tabular part for each family of compounds. The introduction is roughly divided into four parts. The division is not always strictly followed and information from different parts may be mixed together. The four parts contain the following information:

1. statistical data that give the total number of compounds in the family, number of compounds with data at a single temperature, most frequently 298.15 K;
2. a list and characteristics of main laboratories that specialized in the measurement of heat capacity for a particular family of compounds;
3. for multiple sources an explanation is sometimes given why particular data sets were selected for or rejected from the final correlations; this account is presented for most important compounds and in some additional cases where specifications are needed;
4. additional discussion of measurements from certain laboratories where reliability of data is difficult to establish and information in the original source is scarce or doubtful. Supplementary information is given for special cases.

No special attention has been paid in the introductory chapters to the measurements that have been performed at either a single temperature or in a narrow temperature interval; these data are often by-products of excess heat capacity measurements with mixtures (concentration extremes). In the latter investigations the authors did not often pay much attention to sample purity; impurities do not have much effect on excess heat capacities but impact upon the reliability of results for pure substances.

For the sake of clarity, we have sometimes used trivial names of compounds instead of systematic names. The list of all compound names and synonyms used in the compilation is given in the Name Index of Compounds.

We have used acronyms for referring to different laboratories whose names repeatedly appeared in introductory chapters. The list that follows gives an alphabetical list of acronyms and full names of the main laboratories that were engaged in the measurement of heat capacities.

6.2.1. Acronyms of Laboratories

A

ANAZ — Akademia Nauk (Academy of Sciences) Azerbaidzhanskoi SSR, Baku, Azerbaidzhan
ANSM — Akademia Nauk (Academy of Sciences) USSR, Moscow, USSR
APIB — Azerbaidzhanskii Politekh.-Institut, Baku, Azerbaidzhan (Politechnical Institute in Baku)
ASUB — Azerbaidzhan State University, Baku, Azerbaidzhan

B

BAF — Bergakademie Freiberg, Germany
BMB — Bureau of Mines (now see NIPER), Bartlesville, Oklahoma, USA
BSU — Byelorussian State University, Minsk, Byelorussia
BTIM — Byelorussian Technology Institute S.M.Kirova, Minsk, Byelorussia
BYUP — Brigham Young University, Provo, Utah, USA

C

CITP — California Institute of Technology, Pasadena, California, USA
CIUG — Chemistry Institute of Lobachevski State University, Gorki (now Nizhny Novgorod), USSR

D

DCM — Dow Chemical Co., Midland, Michigan, USA
DICP — Dalian Institute of Chemical Physics, Academia Sinica, China

E

EREL — Exxon Research and Equipment Co., Linden, NJ, USA

F

FSO — Faculté des Sciences Orsay, Seine-et-Oise, France
FUAN — Free University, Amsterdam, Netherlands

G

GPI — Groznenski Petroleum Institute, Grozny, Georgia (Oil Institute Academician M.D.Millionshchnikov, Grozny)
GITA — Georgia Institute of Technology, Atlanta, USA

I

ICG — Institute of Chemistry, AN USSR, Gor'kii (now Nizhny Novgorod), USSR
ICLO — The Inorganic Chemistry Laboratory, Oxford, England
ICTP — Institute of Chemical Technology, Prague, Czechoslovakia (now Czech Republic)
IICN — Institute of Inorganic Chemistry, AN USSR, Novosibirsk, USSR
IISB — Indian Institute of Science, Bangalore, India
IITD — Indian Institute of Technology, New Delhi, India
IKNR — Institut Khimii Nevodnykh Raztvorov, AN USSR, Ivanovo, USSR (Institute of Non-Aqueous Solution Chemistry)
IPCL — Institut für Physikalische Chemie, Leuna-Merseburg, Germany
ITN — Institut Teplofiziki, AN USSR, Novosibirsk, USSR
IVTM — Institut Vysokikh Temperatur, AN USSR, Moscow, USSR (Institute of High Temperatures)

J

JHUB — The John Hopkin's University, Baltimore, Maryland, USA

K

KCIW — Kinetic Chemicals Inc., Willmington, Delaware, USA
KGPI — Kurski Gosudarstvenyi Pedagogicheskii Institut, Kursk, USSR
KITH — Kaeltetechnischen Institut der Technische Hochschule Karlsruhe, Germany
KSUK — Kent State University, Kent, Ohio, USA

L

LCPP — Laboratoire de Chimie Physique, Paris, France
LCSP — Laboratoire de Chimie Structurale, Pau, France
LISI — Leningradskii Inzhenerno-Stroitel'nii Institut, Leningrad (now St.Petersburg), USSR (Leningrad Engineering-Architectural Institute)
LSU — Leningrad State University, Leningrad (now St.Petersburg), USSR

M

MCSL — Monsanto Company, St.Louis, Missouri, USA
MGUM — McGill University, Montreal, Canada
MITC — Massachusetts Institute of Technology, Cambridge, USA
MLUH — Martin-Luther University, Halle-Wittenberg, Germany
MRCE — Monsanto Research Corporation, Everett, Massachusetts, USA
MSUM — Moscow State University, Moscow, USSR (Lomonosov State University)

N

NBSB — National Bureau of Standards (from 1990 see NIST), Boulder, Colorado, USA
NBSW — National Bureau of Standards (from 1990 see NIST), Gaithersburg, Maryland, USA
NCLT — National Chemical Laboratory for Industry, Tokyo, Japan
NIPER — National Institute for Petroleum and Energy Research (formerly BMB, see), Bartlesville, Oklahoma, USA
NIST — National Institute of Standards and Technology, Boulder, Colorado and Gaithersburg, Maryland, USA (see formerly NBSB and NBSW)
NPLT — National Physical Laboratory, Teddington, England
NRCO — National Research Council, Ottawa, Canada
NRLW — Naval Research Laboratory, Washington, USA
NWUC — Northwestern University, Xi'an, People Republic China
NWUE — Northwestern University, Evanston, Illinois, USA

O

OCUO — Osaka City University, Osaka, Japan
OSU — Ohio State University, Columbus, USA

P

PASW — Polish Academy of Sciences, Warsaw, Poland
PIK — Polytechnical Institute in Khar'kov, Ukraine
PSC — Pennsylvania State College, Pennsylvania, USA
PTIL — Physical Technology Institute, Leningrad, (now St.Petersburg), USSR
PUP — Princeton University, Princeton, USA

R

RUH — (William Marsh) Rice University, Houston, Texas, USA
RAB — Rumanian Academy, Bucharest, Romania

S

SRIL — Soviet Research Institute of Petroleum Chemistry, Leningrad (now St.Petersburg), USSR
SRNO — Southern Regional Research Laboratory, New Orleans, Louisiana, USA
SUC — Stanford University, California, USA
SUU — State University of Utrecht, Utrecht, The Netherlands

T

THA — Technische Hochschule, Aachen, Germany
TUB — Technical University in Breslau, Germany (now Wroclaw, Poland)

U

UCB — University of California, Berkeley, USA
UCCC — Union Carbide Corporation, Oak Ridge, Tennessee, USA
UCCW — Union Carbide Corporation, South Charleston, West Virginia, USA
UCE — University of Cambridge, England
UGG — University of Goettingen, Germany
UHS — University of Halle/Saale, Germany
ULE — University of London, England
ULS — University of Lund, Sweden
UMAA — University of Michigan, Ann Arbor, USA
UMG — University of Munich, Germany
UME — University of Manchester, England
UMF — University of Miami, Florida, USA
UOE — University of Oxford, England
UOTO — University of Osaka, Toyonaka, Osaka, Japan
USC — University of Sherbrooke, Canada
USE — University of Sulford, England
UWA — University of Vienna, Austria
UWG — University of Wurzburg, Germany

W

WRUC — Western Reserve University, Cleveland, Ohio, USA
WUSL — Washington University, St.Louis, Missouri, USA

Y

YUNH — Yale University, New Haven, Connecticut, USA

6.3. Tables and Deviation Plot

Most of the information on the data and their processing is given for each substance in tables which are described in detail below. Methodology and procedure which led to this presentation of data are described in Chapter 5. The tables for each substance are preceded with name of the substance, its formula, code, and CAS registry number.

The characterization of raw data, their consistency, results of correlation and recommended data are summarized for each substance separately in three to five tables and a deviation plot. A table of *experimental heat capacities* (table type number 1) reviews all primary sources and characterizes briefly experimental conditions and the quality of data. The upper half of the table of *correlated heat capacities* (table type number 2) lists sources selected for establishing the recommended values; the statistical criteria defined in Section 5.2 indicate for both selected and discarded sources how the individual data sets compare with values generated from the correlation equation. The consistency of raw data is graphically demonstrated in the *deviation plot*. The table of correlated heat capacities is not present when the data are available

at only one temperature or when there is only one literature source. The table listing *parameters of polynomial(s)* (table type number 3) obtained by fitting the selected data also gives information on the quality of the overall fit and reliability of the recommended data. The table of *recommended values* (table type number 4) contains discrete heat capacities generated from the listed parameters of polynomials. *Parameters of quasi-polynomial equation* (table type number 5) are presented for substances where application of this relationship is meaningful.

Each table is coded with three numbers separated by periods. The first two numbers are identical with the substance code (see Section 6.1) and the third relates to the type of table (1 to 5). Even when some tables are missing, the numbering related to the type of table is retained.

The symbol C without a subscript specification or the term heat capacity is used in tables whenever we refer both to C_p and C_{sat} at temperatures where the difference between their values is negligible compared with the expected experimental error.

Certain statistics and parameters are listed in the modified E notation. The first part of the number denotes the fractional part which is followed by the exponent to the base 10. The exponent is separated from the fractional part by a plus or a minus sign (e.g. –1.53–5 means $-1.53 \cdot 10^{-5}$).

6.3.1. Experimental Heat Capacities

Each line of the table contains information on one literature source of experimental data. When several distinct data sets were given for the same substance in one publication (for example, parameters of smoothing equations relating to different temperature subintervals or the data obtained from two different calorimeters), there are several lines for one data source, each relating to one data set.

First column: the abbreviated reference in the form YYAAA/BBBM where YY is the last two digits of the year of publication (for a year before 1900 the reference code is preceded by an asterisk), AAA and BBB are the first three letters of the last name of the first and second author (if present), respectively. M is a digit from 1 to 9 distinguishing papers published by the same author(s) within the same year. If the same data set appeared in two or more different publications the reference to the earliest source is given; an appropriate note is given below the table.

For some sources, a footnote is added below the table. In these cases, there is a capital N between the first and second column.

Second column: temperature range of the data set in kelvin.

Third column: number of experimental data points; symbol "eqn" is used in those cases where only parameters of a smoothing equation were presented in the original literature; symbol "S" denotes that the discrete values given in the original literature source were generated from a smoothing equation.

Fourth column: error of measurement, $\sigma_r C_{exp}$, in percent claimed by the author(s); abbreviation "nosp" is used when no specification is given in the original literature.

Fifth column: purity of the substance in percent (given with the same number of significant digits as in the original source) and analytical method used for its determination; the meaning of the abbreviations used is as follows: "anal"– analytical (used when the analytical method was not specified), "chrom"– gas or liquid chromatography, "estim"– the purity was estimated by the author(s), "melpt"– determination of impurities from the melting point depression.

Sixth column: type of heat capacity reported in the original literature; C_p—isobaric heat capacity, C_{sat}—saturation heat capacity, C_{avg}– average heat capacity determined over a temperature range usually greater than 10 K.

Seventh column: type of calorimetric method used for determining the data and reference to the publication where the instrument is described. The coding used for classification of experimental techniques is introduced in Table 2 and the individual types of calorimeters are summarized in Table 3 (both in Chapter 3). The criteria for classifying heat capacity calorimeters are discussed in Section 3.1. All references to calorimeters listed in tables of experimental heat capacities are summarized in Table 4.

More information on experimental data is given in Section 5.1.

6.3.2. Correlated Heat Capacities

This table contains information on the results of the correlation presented for the individual data sets. The statistics for the selected and rejected data sets are listed in the upper and lower half of the table, respectively. The meaning of the columns in the *upper part* of the table is as follows.

First column: the abbreviated reference (the same as in the table of experimental heat capacities).

Second column: temperature range (in kelvin) in which the data from a particular source were included in the correlation.

Third column: number of values used in the final determination of the correlation parameters.

The entries in the second and third columns are identical to those in the table of experimental heat capacities when the whole data set was included in the correlation; they differ if part of the data was discarded.

Fourth column: percentage error, $\sigma_r C$, used in Eq. (V-2) to estimate the variance of individual data points. This value is either $\sigma_r C_{exp}$ (column 4 in the table of experimental heat capacities) or is assigned by the evaluator in cases when no error is specified in the original source or the author's estimate does not seem to be realistic. When $\sigma_r C$ was assigned or modified by the evaluator, the value is followed by the sign #.

Fifth column: average weighted deviation d_w defined by Eq. (V-7).

Sixth column: average deviation d, defined by Eq. (V-8), divided by R (dimensionless).

Seventh column: average percentage deviation d_r defined by Eq. (V-9).

Eighth column: bias of the data set d_b, defined by Eq. (V-10), divided by R (dimensionless).

Ninth column: the difference between the number of experimental points with positive and negative deviation from the recommended values (denoted by +/–).

In the *lower part* of the table, the quantities d/R, d_r, d_b/R and +/– are presented in parenthesis for each reference rejected from the final correlation.

In some cases, the correlations for isobaric and saturation heat capacities were performed separately. We give, however, only one table of correlated heat capacities for these compounds as the selection of data sources did not differ and statistical values were practically identical in both correlations.

More information on the evaluation and selection processes can be found in Section 5.2.

6.3.3. Parameters of Polynomials

This table gives characteristics of the final correlation of the selected data in the upper part and, the corresponding parameters of the polynomial(s) in the lower part.

The *upper part* consists of two lines when both isobaric and saturation heat capacities are tabulated and of only one line when no distinction is made between the two heat capacities. The following items are listed.

First column: type of heat capacity listed — C_p and C_{sat} denote isobaric and saturation heat capacities, respectively. The C is used when no distinction was made between the two types of heat capacities (see Section 5.4.)

Second column: the total number of all experimental data points available.

Third column: the total number of experimental data points used in the correlation.

Fourth column: the standard weighted deviation s_w defined by Eqns. (V-1) and (V-3).

Fifth column: standard deviation s, defined by Eq. (V-4), divided by R (dimensionless).

Sixth column: standard percentage deviation s_r defined by Eq. (V-5).

Seventh column: bias s_b, defined by Eq. (V-6), divided by R (dimensionless).

Eighth column: the overall difference between the numbers of experimental points with positive and negative deviations from the recommended values (denoted by +/–).

The parameters of the cubic spline polynomials describing individual subintervals of the temperature range of the selected data are listed in the *lower part* of the table. When the isobaric and saturation heat capacities are distinguished, two sets of parameters are listed separately, the first set relating to the temperature correlation of C_p and the second to that of C_{sat}. When the whole temperature range of experimental data is described by only one equation the parameters were obtained by simple unconstrained fitting using a polynomial of third or lower degree. The meaning of the individual columns is as follows:

First column: temperature subinterval in kelvin to which the listed parameters relate.

Second to fifth columns: parameters of the polynomial defined by Eq. (V-11) valid in the given subinterval. Dimension of the parameters is K^{-j}.

Sixth column: level of uncertainty assigned by the evaluators to the data generated from the polynomial in the given temperature subinterval. This characteristic expresses the expected overall uncertainty of the recommended data and reflects both the uncertainty in the experimental values and possible error due to the fitting procedure. The following levels of uncertainty were assigned:

I	excellent data (uncertainty below 0.1 percent)
II	highly reliable data (uncertainty below 0.3 percent)
III	reliable data (uncertainty below 0.5 percent)
IV	medium quality data (uncertainty below 1 percent)
V	data of low reliability (uncertainty below 3 percent)
VI	very unreliable data with a possibility of gross systematic errors (uncertainty above 3 percent).

The level of uncertainty assigned to individual subintervals for cubic splines often differs due to the unequal reliability of experimental data in different parts of the temperature range. On the other hand in certain cases one set of parameters was used for describing two (or exceptionally three) experimental data sets of different accuracy, which related to different temperature ranges. Then the level of uncertainty assigned to recommended data relates always to the data set of lower quality; in reality the recommended data are more reliable than indicated at temperatures where the experimental data set of higher quality was available. The reader can obtain information regarding changes of reliability within the temperature interval of recommended data from the table of Correlated Heat Capacities.

More details on fitting data with polynomials can be found in Section 5.3.1.

6.3.4. Recommended Values

This table lists recommended specific and molar heat capacities generated from the parameters of the polynomials at typical temperatures 273.15 and 298.15 K (provided they lie inside the interval of experimental data) and over the whole temperature range of the selected experimental data. Isobaric and saturation heat capacities are tabulated when the parameters for both C_p and C_{sat} were determined, otherwise only one data set is presented. The number of significant digits is determined by the level of uncertainty of the recommended values.

For some compounds where most of experimental data are available above the normal boiling temperature the recommended isobaric and saturation heat capacities exhibit small differences in the temperature range where both quantities are in other cases equal. This artifact is exclusively due to the fitting procedure.

6.3.5. Parameters of the Quasi-Polynomial Equation

The quasi-polynomial equation (V-12) is useful as a simple expression permitting extrapolations to higher temperatures (see Section 5.3.2. for details). The quasi-polynomial fit is performed only for C_p data as its main application was in the calculation of enthalpy and entropy differences.

The table is organized analogously to the table presenting parameters of polynomials; the *upper part* of the table is identical. The items tabulated in the *lower part* have the following meaning.

First column: temperature interval in kelvin to which the listed parameters relate. This interval is not necessarily identical with the temperature range of the representation by polynomials.

Second column: critical temperature in kelvin

Third to eighth columns: four or six parameters of the quasi-polynomial equation (m = 1 or 3). The parameters are dimensionless.

Ninth column: level of uncertainty assigned by the evaluators to the data generated from the quasi-polynomial equation within the temperature range of the experimental data. When using the equation outside this range, the uncertainty decreases with the length of the extrapolation.

6.3.6. Deviation Plots

An overview of the deviations from the recommended values for all experimental data (both included in and rejected from the final correlation) measured by various authors is presented in graphical form in the deviation plots. The temperature is plotted along the x-axis and the relative percentage deviation for individual data points along the y-axis. Data from different sources are distinguished by different symbols. Points that lie outside the range of the ordinate in the plot are accompanied by the numerical value of the deviation. Some points that overlap each other or the accompanying figures are omitted. When too many data points were available some less important sets and values exhibiting large deviations from the recommended data were not included.

7. References

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Formula Index of Compounds

The formula index of compounds lists all compounds for which data were compiled and evaluated. Compounds are sorted in the order of empirical formulas. The empirical formula is listed on the first line. The second line introduced by the sign • gives the name of a compound and the Chemical Abstracts Service Registry Number (CAS RN) enclosed in brackets. The next line(s), if present, gives synonyms, common names or commercial names. The last line for each compound lists the group-member number. The system of dividing compounds into groups is described in detail in the Section 6.1. The first two-digit number indicates the group, and the second three-digit number denotes the serial number of a compound inside the group. Tables in the compilation are coded with three numbers separated by full stops. The first two numbers are identical with the compound group and member number.

If there are more compounds of the same empirical formula, they are listed under a common formula and each different compound is introduced by the sign •.

For geometric isomers which are common among alkenes the symbols (*Z*) and (*E*) are used to identify similar groups either on the same side of the double bond or across from the double bond. For simple systems (*Z*) and (*E*) are equivalent to *cis* and *trans*.

BrIn
• Indium bromide (InBr) [14280-53-6]
Group-member nr.: 02-017

Br_2
• Bromine [7726-95-6]
Group-member nr.: 01-003

Br_2Sn
• Tin bromide ($SnBr_2$) [10031-24-0]
Group-member nr.: 02-018

Br_4Sn
• Tetrabromostannane [7789-67-5]
Tin(IV) bromide
Tin tetrabromide
Group-member nr.: 02-019

$CBrCl_3$
• Bromotrichloromethane [75-62-7]
Group-member nr.: 25-001

$CBrF_3$
• Bromotrifluoromethane [75-63-8]
R13B1
Group-member nr.: 25-002

CBr_4
• Tetrabromomethane [558-13-4]
Carbon tetrabromide
Perbromomethane
Group-member nr.: 23-001

$CClF_3$
• Chlorotrifluoromethane [75-72-9]
R13
Group-member nr.: 25-003

$CClN_3O_6$
• Chlorotrinitromethane [1943-16-4]
Group-member nr.: 64-001

CCl_2F_2
• Dichlorodifluoromethane [75-71-8]
R12
Group-member nr.: 25-004

CCl_2O
• Carbonic dichloride [75-44-5]
Phosgene
Group-member nr.: 02-020

CCl_3F
• Trichlorofluoromethane [75-69-4]
R11
Group-member nr.: 25-005

CCl_4
• Tetrachloromethane [56-23-5]
Carbon tetrachloride
Perchloromethane
Group-member nr.: 22-001

CD_4
• Methane-d_4 [558-20-3]
Deuteromethane
Group-member nr.: 11-001

CF_2O
• Carbonic difluoride [353-50-4]
Carbonyl fluoride
Group-member nr.: 02-021

CF_4
• Tetrafluoromethane [75-73-0]
Carbon tetrafluoride
Perfluoromethane
R14
Group-member nr.: 21-001

$CHBr_3$
• Tribromomethane [75-25-2]
Bromoform
Methenyl tribromide
Group-member nr.: 23-002

$CHClF_2$
• Chlorodifluoromethane [75-45-6]
R22
Group-member nr.: 25-006

$CHCl_2F$
• Dichlorofluoromethane [75-43-4]
R21
Group-member nr.: 25-007

$CHCl_3$
• Trichloromethane [67-66-3]
Chloroform
Methylidyne trichloride
Group-member nr.: 22-002

CHF_3
• Trifluoromethane [75-46-7]
Fluoroform
R23
Group-member nr.: 21-002

CHF_3S
• Trifluoromethanethiol [1493-15-8]
Group-member nr.: 64-002

CHN
• Hydrocyanic acid [74-90-8]
Hydrogen cyanide
Group-member nr.: 02-022

$CHNaO_2$
- Sodium salt formic acid [141-53-7]
  Sodium formate
  Natrium formate
  Group-member nr.: 74-001

CH_2Br_2
- Dibromomethane [74-95-3]
  Methylene dibromide
  Group-member nr.: 23-003

CH_2Cl_2
- Dichloromethane [75-09-2]
  Methylene dichloride
  Group-member nr.: 22-003

CH_2I_2
- Diiodomethane [75-11-6]
  Methylene diiodide
  Group-member nr.: 24-001

CH_2N_2
- Cyanamide [420-04-2]
  Group-member nr.: 34-001

CH_2O_2
- Formic acid [64-18-6]
  Methanoic acid
  Hydrogencarboxylic acid
  Group-member nr.: 44-001

CH_2S_3
- Trithiocarbonic acid [594-08-1]
  Carbon sulfide dihydrosulfide
  Group-member nr.: 02-023

CH_3Br
- Bromomethane [74-83-9]
  Methyl bromide
  Group-member nr.: 23-004

CH_3Cl
- Chloromethane [74-87-3]
  Methyl chloride
  Group-member nr.: 22-004

CH_3ClFOP
- Methylphosphonic chloride fluoride [753-71-9]
  Methylphosphonic chlorofluoride
  Group-member nr.: 72-001

CH_3Cl_2OP
- Methylphosphonic dichloride [676-97-1]
  Group-member nr.: 72-002

CH_3D
- Methane-*d* [676-49-3]
  Monodeuteromethane
  Group-member nr.: 11-002

CH_3DO
- Methanol-*d* [1455-13-6]
  Monodeuteromethanol
  Group-member nr.: 42-001

CH_3F_2OP
- Methylphosphonic difluoride [676-99-3]
  Group-member nr.: 72-003

CH_3I
- Iodomethane [74-88-4]
  Methyl iodide
  Group-member nr.: 24-002

CH_3NO
- Formamide [75-12-7]
  Methanamide
  Group-member nr.: 62-001

CH_3NO_2
- Nitromethane [75-52-5]
  Group-member nr.: 62-002

CH_3NO_3
- Methyl ester nitric acid [598-58-3]
  Methyl nitrate
  Group-member nr.: 62-003

CH_4
- Methane [74-82-8]
  Group-member nr.: 11-003

CH_4N_2O
- Urea [57-13-6]
  Carbamide
  Group-member nr.: 62-004

CH_4O
- Methanol [67-56-1]
  Methyl alcohol
  Carbinol
  Wood alcohol
  Group-member nr.: 42-002

CH_4S
- Methanethiol [74-93-1]
  Methyl mercaptan
  Group-member nr.: 52-001

CH_5N
- Methanamine [74-89-5]
  Methylamine
  Aminomethane
  Group-member nr.: 31-001

CH_6N_2
- Methylhydrazine [60-34-4]
  Monomethylhydrazine
  Group-member nr.: 34-002

CO
- Carbon monoxide [630-08-0]
  Group-member nr.: 02-024

COS
- Carbon oxide sulfide [463-58-1]
  Carbonyl sulfide
  Group-member nr.: 02-025

CO_2
- Carbon dioxide [124-38-9]
  Group-member nr.: 02-026

CS_2
- Carbon disulfide [75-15-0]
  Group-member nr.: 02-027

CSe_2
- Carbon selenide (CSe_2) [506-80-9]
  Group-member nr.: 02-028

$C_2Br_2D_4$
- 1,2-Dibromoethane-1,1,2,2-d_4 [22581-63-1]
  1,2-Dibromotetradeuteroethane
  Group-member nr.: 23-005

$C_2Br_2F_4$
- 1,2-Dibromo-1,1,2,2-tetrafluoroethane [124-73-2]
  R114B2
  Group-member nr.: 25-008

$C_2Br_3D_3$
- 1,1,2-Tribromoethane-1,2,2-d_3 [unknown]
  Group-member nr.: 23-006

C_2ClF_3
- Chlorotrifluoroethene [79-38-9]
  Chlorotrifluoroethylene
  Group-member nr.: 25-009

C_2ClF_5
- Chloropentafluoroethane [76-15-3]
  R115
  Group-member nr.: 25-010

$C_2Cl_2F_4$
- 1,2-Dichloro-1,1,2,2-tetrafluoroethane [76-14-2]
  sym-Dichlorotetrafluoroethane
  Fluorocarbon-114
  R114
  Group-member nr.: 25-012
- Dichlorotetrafluoroethane (unspecified isomer) [1320-37-2]
  Group-member nr.: 25-011

$C_2Cl_3F_3$
- 1,1,1-Trichloro-2,2,2-trifluoroethane [354-58-5]
  Group-member nr.: 25-013
- 1,1,2-Trichloro-1,2,2-trifluoroethane [76-13-1]
  R113
  Group-member nr.: 25-014

C_2Cl_4
- Tetrachloroethene [127-18-4]
  Perchloroethylene
  Group-member nr.: 22-005

$C_2Cl_4F_2$
- 1,1,2,2-Tetrachloro-1,2-difluoroethane [76-12-0]
  sym-Tetrachlorodifluoroethane
  R112
  Group-member nr.: 25-015

$C_2F_2O_2$
- Ethanedioyl difluoride [359-40-0]
  Oxalyl difluoride
  Group-member nr.: 61-001

C_2F_3N
- Trifluoroacetonitrile [353-85-5]
  Trifluoroethanenitrile
  Trifluoromethyl cyanide
  Group-member nr.: 64-003

C_2F_4
- Tetrafluoroethene [116-14-3]
  Perfluoroethylene
  Group-member nr.: 21-003

C_2F_4O
- Trifluoroacetyl fluoride [354-34-7]
  Group-member nr.: 61-002

C_2F_6
- Hexafluoroethane [76-16-4]
  Perfluoroethane
  Group-member nr.: 21-004

$C_2HBrClF_3$
- 1-Bromo-2-chloro-1,1,2-trifluoroethane [354-06-3]
  Group-member nr.: 25-016
- 2-Bromo-2-chloro-1,1,1-trifluoroethane [151-67-7]
  Halothane
  Group-member nr.: 25-017

$C_2HBr_2D_3$
- 1,2-Dibromoethane-1,1,2-d_3 [117164-17-7]
  Group-member nr.: 23-007

$C_2HBr_3D_2$
- 1,1,2-Tribromoethane-2,2-d_2 [unknown]
  Group-member nr.: 23-008

C_2HCl_3
- Trichloroethene [79-01-6]
  Trichloroethylene
  Group-member nr.: 22-006

$C_2HCl_3F_2$
- 1,1,2-Trichloro-1,2-difluoroethane [354-15-4]
  R122
  Group-member nr.: 25-018

C_2HCl_3O
- Trichloroacetaldehyde [75-87-6]
  Trichloroethanal
  Chloral
  Group-member nr.: 61-003

$C_2HCl_3O_2$
- Trichloroacetic acid [76-03-9]
  Trichloroethanoic acid
  Group-member nr.: 61-004

C_2HCl_5
- Pentachloroethane [76-01-7]
  Pentalin
  Group-member nr.: 22-007

$C_2H_2Br_2D_2$
- 1,2-Dibromoethane-1,1-d_2 [unknown]
  Group-member nr.: 23-009
- 1,2-Dibromoethane-1,2-d_2 [unknown]
  Group-member nr.: 23-010

$C_2H_2Br_3D$
- 1,1,2-Tribromoethane-1-*d* [unknown]
  Group-member nr.: 23-011
- 1,1,2-Tribromoethane-2-*d* [unknown]
  Group-member nr.: 23-012

$C_2H_2Br_4$
- 1,1,2,2-Tetrabromoethane [79-27-6]
  sym-Tetrabromoethane
  Acetylene tetrabromide
  Group-member nr.: 23-013

$C_2H_2Cl_2$
- 1,1-Dichloroethene [75-35-4]
  1,1-Dichloroethylene
  Vinylidene chloride
  Group-member nr.: 22-008
- 1,2-Dichloroethene [540-59-0]
  1,2-Dichloroethylene (unspecified stereoisomer)
  Group-member nr.: 22-009
- (*E*)-1,2-Dichloroethene [156-60-5]
  trans-1,2-Dichloroethene
  trans-1,2-Dichloroethylene
  Group-member nr.: 22-010
- (*Z*)-1,2-Dichloroethene [156-59-2]
  cis-1,2-Dichloroethene
  cis-1,2-Dichloroethylene
  Group-member nr.: 22-011

$C_2H_2Cl_2F_2$
- 1,1-Dichloro-1,2-difluoroethane [1842-05-3]
  R132
  Group-member nr.: 25-019

$C_2H_2Cl_2O_2$
- Dichloroacetic acid [79-43-6]
  Dichloroethanoic acid
  Group-member nr.: 61-005

$C_2H_2Cl_4$
- 1,1,1,2-Tetrachloroethane [630-20-6]
  Group-member nr.: 22-012
- 1,1,2,2-Tetrachloroethane [79-34-5]
  sym-Tetrachloroethane
  Acetylene tetrachloride
  Group-member nr.: 22-013

C_2H_3Br
- Bromoethene [593-60-2]
  Bromoethylene
  Vinyl bromide
  Group-member nr.: 23-014

$C_2H_3Br_2D$
- 1,2-Dibromoethane-*d* [unknown]
  Group-member nr.: 23-015

$C_2H_3Br_3$
- 1,1,2-Tribromoethane [78-74-0]
  Group-member nr.: 23-016

C_2H_3Cl
- Chloroethene [75-01-4]
  Vinyl chloride
  Group-member nr.: 22-014

$C_2H_3ClF_2$
- 1-Chloro-1,1-difluoroethane [75-68-3]
  R142
  Group-member nr.: 25-020

C_2H_3ClO
- Acetyl chloride [75-36-5]
  Ethanoyl chloride
  Group-member nr.: 61-006

$C_2H_3ClO_2$
- Chloroacetic acid [79-11-8]
  Chloroethanoic acid
  Group-member nr.: 61-007

$C_2H_3Cl_3$
- 1,1,1-Trichloroethane [71-55-6]
  Methylchloroform
  Group-member nr.: 22-015
- 1,1,2-Trichloroethane [79-00-5]
  β-Trichloroethane
  Group-member nr.: 22-016

$C_2H_3Cl_3Si$
- Trichloroethenylsilane [75-94-5]
  Trichlorovinylsilane
  Group-member nr.: 71-001

$C_2H_3F_3$
- 1,1,1-Trifluoroethane [420-46-2]
  Group-member nr.: 21-005

$C_2H_3F_3O$
- 2,2,2-Trifluoroethanol [75-89-8]
  Group-member nr.: 61-008

C_2H_3N
- Acetonitrile [75-05-8]
  Ethanenitrile
  Group-member nr.: 32-002

C_2H_4
- Ethene [74-85-1]
  Ethylene
  Group-member nr.: 13-001

C_2H_4BrCl
- 1-Bromo-2-chloroethane [107-04-0]
  Ethylene chlorobromide
  Group-member nr.: 25-021

$C_2H_4Br_2$
- 1,2-Dibromoethane [106-93-4]
  Ethylene dibromide
  Group-member nr.: 23-017

$C_2H_4Cl_2$
- 1,1-Dichloroethane [75-34-3]
  Ethylidene dichloride
  Group-member nr.: 22-017
- 1,2-Dichloroethane [107-06-2]
  Ethylene dichloride
  Group-member nr.: 22-018

$C_2H_4D_2O_2$
- 1,2-Ethanediol-d_2 [2219-52-5]
  Dideutero-1,2-ethanediol
  Dideuteroethylene glycol
  Group-member nr.: 42-003

C_2H_4O
- Acetaldehyde [75-07-0]
  Ethanal
  Group-member nr.: 43-001
- Oxirane [75-21-8]
  Epoxyethane
  Ethylene oxide
  Group-member nr.: 46-001

$C_2H_4O_2$
- Acetic acid [64-19-7]
  Ethanoic acid
  Methanecarboxylic acid
  Vinegar acid
  Group-member nr.: 44-002
- Methyl formate [107-31-3]
  Methyl methanoate
  Group-member nr.: 45-001

C_2H_5Br
- Bromoethane [74-96-4]
  Ethyl bromide
  Group-member nr.: 23-018

C_2H_5Cl
- Chloroethane [75-00-3]
  Ethyl chloride
  Group-member nr.: 22-019

$C_2H_5Cl_3Si$
- Trichloroethylsilane [115-21-9]
  Group-member nr.: 71-002

C_2H_5DO
- Ethanol-*d* [925-93-9]
  Monodeuteroethanol
  Group-member nr.: 42-004

C_2H_5I
- Iodoethane [75-03-6]
  Ethyl iodide
  Group-member nr.: 24-003

C_2H_5N
- Aziridine [151-56-4]
  Ethylene imine
  Group-member nr.: 33-001

C_2H_5NO
- Acetamide [60-35-5]
  Ethanamide
  Group-member nr.: 62-005
- *N*-Methylformamide [123-39-7]
  Group-member nr.: 62-006

$C_2H_5NO_2$
- Nitroethane [79-24-3]
  Group-member nr.: 62-007

$C_2H_5NO_3$
- Ethyl nitrate [625-58-1]
  Ethyl ester nitric acid
  Group-member nr.: 62-008

C_2H_6
- Ethane [74-84-0]
  Group-member nr.: 11-004

C_2H_6Cd
- Dimethylcadmium [506-82-1]
  Group-member nr.: 73-001

$C_2H_6Cl_2Si$
- Dichloroethylsilane [1789-58-8]
  Group-member nr.: 71-003

C_2H_6O
- Ethanol [64-17-5]
  Ethyl alcohol
  Grain alcohol
  Group-member nr.: 42-005
- Oxydimethane [115-10-6]
  Dimethyl ether
  Methyl ether
  Methyl oxide
  Wood ether
  Group-member nr.: 41-001

C_2H_6OS
- Sulfinyldimethane [67-68-5]
  Dimethyl sulfoxide
  DMSO
  Group-member nr.: 63-001

$C_2H_6O_2$
- 1,2-Ethanediol [107-21-1]
  Ethylene glycol
  Glycol
  Group-member nr.: 42-006

$C_2H_6O_2S$
- Sulfonyldimethane [67-71-0]
  Dimethyl sulfone
  Group-member nr.: 63-002

C_2H_6S
- Ethanethiol [75-08-1]
  Ethyl mercaptan
  Group-member nr.: 52-002
- Thiodimethane [75-18-3]
  Dimethyl sulfide
  Group-member nr.: 51-001

$C_2H_6S_2$
- 2,3-Dithiabutane [624-92-0]
  Dimethyl disulfide
  Methyl disulfide
  Group-member nr.: 51-002

C_2H_6Se
- Selenodimethane [593-79-3]
  Dimethyl selenide
  Methyl selenide
  Group-member nr.: 73-002

$C_2H_6Se_2$
- Dimethyl diselenide [7101-31-7]
  Methyl diselenide
  Group-member nr.: 73-003

C_2H_6Zn
- Dimethylzinc [544-97-8]
  Group-member nr.: 73-004

C_2H_7N
- Ethanamine [75-04-7]
  Ethylamine
  Group-member nr.: 31-002
- *N*-Methylmethanamine [124-40-3]
  Dimethylamine
  Group-member nr.: 31-003

$C_2H_8N_2$
- 1,1-Dimethylhydrazine [57-14-7]
  unsym-Dimethylhydrazine
  Group-member nr.: 34-003
- 1,2-Dimethylhydrazine [540-73-8]
  sym-Dimethylhydrazine
  Group-member nr.: 34-004
- 1,2-Ethanediamine [107-15-3]
  Ethylenediamine
  1,2-Diaminoethane
  Group-member nr.: 31-004

$C_2H_8N_2O_3$
- Nitrate ethylamine [22113-86-6]
  Ethylammonium nitrate
  Group-member nr.: 62-009

$C_2H_{11}B_2N$
- (Dimethylamino)diborane(6) [22580-01-4]
  Group-member nr.: 72-004

C_2N_2
- Ethanedinitrile [460-19-5]
  Cyanogen
  Group-member nr.: 32-001

C_3F_6O
- 1,1,1,3,3,3-Hexafluoro-2-propanone [684-16-2]
  Hexafluoroacetone
  Perfluoroacetone
  Group-member nr.: 61-009

C_3F_8
- Octafluoropropane [76-19-7]
  Perfluoropropane
  Group-member nr.: 21-006

$C_3H_2ClF_5$
- 1-Chloro-1,1,3,3,3-pentafluoropropane [460-92-4]
  Group-member nr.: 25-022

$C_3H_2Cl_3F_3$
- 1,1,1-Trichloro-3,3,3-trifluoropropane [7125-84-0]
  Group-member nr.: 25-023

$C_3H_2N_2$
- Propanedinitrile [109-77-3]
  Malononitrile
  Dicyanomethane
  Group-member nr.: 32-003

$C_3H_3Cl_2F_3$
- 3,3-Dichloro-1,1,1-trifluoropropane [460-69-5]
  Group-member nr.: 25-024

$C_3H_3Cl_3O_2$
- Methyl trichloroacetate [598-99-2]
  Methyl ester trichloroacetic acid
  Group-member nr.: 61-010

C_3H_3N
- 2-Propenenitrile [107-13-1]
  Acrylonitrile
  Vinyl cyanide
  Group-member nr.: 32-004

C_3H_3NO
- Isoxazole [288-14-2]
  Group-member nr.: 62-010
- Oxazole [288-42-6]
  Group-member nr.: 62-011

C_3H_3NS
- Thiazole [288-47-1]
  Group-member nr.: 64-004

$C_3H_3N_3$
- 1,3,5-Triazine [290-87-9]
  sym-Triazine
  Group-member nr.: 33-002

$C_3H_4ClF_3$
- 3-Chloro-1,1,1-trifluoropropane [460-35-5]
  Group-member nr.: 25-025

$C_3H_4Cl_2O_2$
- Methyl dichloroacetate [116-54-1]
  Methyl ester dichloroacetic acid
  Group-member nr.: 61-011

$C_3H_4Cl_3NSi$
- 3-Trichlorosilylpropanenitrile [1071-22-3]
  Group-member nr.: 71-004

$C_3H_4Cl_4$
- 1,1,1,3-Tetrachloropropane [1070-78-6]
  Group-member nr.: 22-020

$C_3H_4N_2$
- 1*H*-Imidazole [288-32-4]
  1,3-Diazole
  Glyoxaline
  Group-member nr.: 33-003
- 1*H*-Pyrazole [288-13-1]
  1,2-Diazole
  Group-member nr.: 33-004

$C_3H_4N_2O$
- 2-Cyanoacetamide [107-91-5]
  Group-member nr.: 62-012

$C_3H_4O_2$
- 2-Oxetanone [57-57-8]
  β-Propiolactone
  Hydracrylolactone
  USAN
  Group-member nr.: 47-001
- 2-Propenoic acid [79-10-7]
  Acrylic acid
  Acroleic acid
  Group-member nr.: 44-003

$C_3H_4O_3$
- 1,3-Dioxolan-2-one [96-49-1]
  Cyclic ethylene ester carbonic acid
  Ethylene carbonate
  Group-member nr.: 47-002

C_3H_5Br
- 3-Bromo-1-propene [106-95-6]
  Allyl bromide
  Group-member nr.: 23-019

$C_3H_5Br_3$
- 1,2,3-Tribromopropane [96-11-7]
  Group-member nr.: 23-020

C_3H_5Cl
- 3-Chloro-1-propene [107-05-1]
  3-Chloropropene
  Allyl chloride
  Group-member nr.: 22-021

C_3H_5ClO
- Propanoyl chloride [79-03-8]
  Propionyl chloride
  Group-member nr.: 61-012

$C_3H_5ClO_2$
- Methyl chloroacetate [96-34-4]
  Methyl ester chloroacetic acid
  Group-member nr.: 61-013

$C_3H_5Cl_3$
- 1,2,3-Trichloropropane [96-18-4]
  Group-member nr.: 22-022

$C_3H_5D_3O_3$
- 1,2,3-Propanetriol-*O*,*O*,*O*-d_3 [7325-16-8]
  Glycerol-*O*,*O*,*O*-d_3
  Trideuteroglycerol
  Group-member nr.: 42-007

C_3H_5N
- Propanenitrile [107-12-0]
  Propionitrile
  Ethyl cyanide
  Group-member nr.: 32-005

C_3H_5NO
- 2-Propenamide [79-06-1]
  Acrylamide
  Group-member nr.: 62-013

$C_3H_5NO_4$
- Methyl ester nitroacetic acid [2483-57-0]
  Methyl nitroacetate
  Group-member nr.: 62-014

C_3H_5NS
- Isothiocyanatoethane [542-85-8]
  Ethyl isothiocyanate
  Group-member nr.: 64-005

$C_3H_5NaO_2$
- Sodium salt propanoic acid [137-40-6]
  Sodium propanoate
  Natrium propionate
  Group-member nr.: 74-002

C_3H_6
- Cyclopropane [75-19-4]
  Trimethylene
  Group-member nr.: 12-001
- 1-Propene [115-07-1]
  Propylene
  Group-member nr.: 13-002

$C_3H_6Br_2$
- 1,2-Dibromopropane [78-75-1]
  Propylene bromide
  Group-member nr.: 23-021
- 1,3-Dibromopropane [109-64-8]
  Trimethylene bromide
  Group-member nr.: 23-022

$C_3H_6Cl_2$
- 1,2-Dichloropropane [78-87-5]
  Propylene chloride
  Group-member nr.: 22-023
- 1,3-Dichloropropane [142-28-9]
  Trimethylene dichloride
  Group-member nr.: 22-024
- 2,2-Dichloropropane [594-20-7]
  Isopropylidene chloride
  Group-member nr.: 22-025

$C_3H_6F_4N_2$
- *N,N,N',N'*-Tetrafluoro-1,2-propanediamine [15403-25-5]
  Group-member nr.: 64-006

$C_3H_6N_2O_4$
- 2,2-Dinitropropane [595-49-3]
  Group-member nr.: 62-015

C_3H_6O
- Methyloxirane [75-56-9]
  1,2-Epoxypropane
  Propene oxide
  Group-member nr.: 46-002
- Oxetane [503-30-0]
  Trimethylene oxide
  Group-member nr.: 46-003
- Propanal [123-38-6]
  Propionaldehyde
  Group-member nr.: 43-003
- 2-Propanone [67-64-1]
  Dimethyl ketone
  Acetone
  Group-member nr.: 43-004
- 2-Propen-1-ol [107-18-6]
  Allyl alcohol
  Group-member nr.: 42-008

$C_3H_6O_2$
- 1,3-Dioxolane [646-06-0]
  Group-member nr.: 46-004
- Ethyl formate [109-94-4]
  Ethyl methanoate
  Group-member nr.: 45-002
- Methyl acetate [79-20-9]
  Methyl ethanoate
  Group-member nr.: 45-003
- Propanoic acid [79-09-4]
  Propionic acid
  Methylacetic acid
  Group-member nr.: 44-004

$C_3H_6O_2S$
- 3-Mercaptopropanoic acid [107-96-0]
  3-Sulfanylpropionic acid
  Group-member nr.: 63-003

$C_3H_6O_3$
- Dimethyl carbonate [616-38-6]
  Methyl carbonate
  Group-member nr.: 45-004
- (*R,S*)-2-Hydroxypropanoic acid [598-82-3]
  Lactic acid (racemic)
  Group-member nr.: 47-003
- 1,3,5-Trioxane [110-88-3]
  sym-Trioxane
  Group-member nr.: 46-005

C_3H_6S
- Thietane [287-27-4]
  Thiacyclobutane
  Trimethylene sulfide
  Group-member nr.: 53-001

C_3H_7Br
- 1-Bromopropane [106-94-5]
  Propyl bromide
  Group-member nr.: 23-023
- 2-Bromopropane [75-26-3]
  Isopropyl bromide
  Group-member nr.: 23-024

C_3H_7Cl
- 1-Chloropropane [540-54-5]
  Propyl chloride
  Group-member nr.: 22-026

C_3H_7I
- 1-Iodopropane [107-08-4]
  Propyl iodide
  Group-member nr.: 24-004

$C_3H_7N_2$
- Cyclopropanamine [765-30-0]
  Cyclopropylamine
  Group-member nr.: 31-005

C_3H_7NO
- *N*, *N*-Dimethylformamide [68-12-2]
  N, *N*-Dimethylmethanamide
  Group-member nr.: 62-016

$C_3H_7NO_2$
- Ethyl ester carbamic acid [51-79-6]
  Ethyl carbamate
  Ethyl urethane
  Group-member nr.: 62-017

$C_3H_7NO_3$
- 1-Methylethyl ester nitric acid [1712-64-7]
  Isopropyl nitrate
  Group-member nr.: 62-018

C_3H_8
- Propane [74-98-6]
  Group-member nr.: 11-005

C_3H_8O
- 1-Propanol [71-23-8]
  Propyl alcohol
  Group-member nr.: 42-009
- 2-Propanol [67-63-0]
  Isopropyl alcohol
  Group-member nr.: 42-010

$C_3H_8O_2$
- Dimethoxymethane [109-87-5]
  2,4-Dioxapentane
  Formaldehyde dimethyl acetal
  Methylal
  Group-member nr.: 41-002
- 2-Methoxyethanol [109-86-4]
  Methyl cellosolve
  Glycol monomethyl ether
  Group-member nr.: 47-004
- 1,2-Propanediol [57-55-6]
  Propylene glycol
  Group-member nr.: 42-011

$C_3H_8O_3$
- 1,2,3-Propanetriol [56-81-5]
  Glycerol
  Glycyl alcohol
  Glycerine
  Group-member nr.: 42-012

C_3H_8S
- (Methylthio)ethane [624-89-5]
  Ethyl methyl sulfide
  Group-member nr.: 51-003
- 1-Propanethiol [107-03-9]
  1-Propyl mercaptan
  Group-member nr.: 52-003
- 2-Propanethiol [75-33-2]
  Isopropyl mercaptan
  Group-member nr.: 52-004

C_3H_9Al
- Trimethylaluminium [75-24-1]
  Group-member nr.: 73-005

C_3H_9As
- Trimethylarsine [593-88-4]
  Group-member nr.: 73-006

C_3H_9B
- Trimethylborane [593-90-8]
  Group-member nr.: 72-005

C_3H_9Ga
- Trimethylgallium [1445-79-0]
  Group-member nr.: 73-007

C_3H_9N
- *N*, *N*-Dimethylmethanamine [75-50-3]
  Trimethylamine
  Group-member nr.: 31-006
- 1-Propanamine [107-10-8]
  n-Propylamine
  Group-member nr.: 31-007
- 2-Propanamine [75-31-0]
  Isopropylamine
  Group-member nr.: 31-008

$C_3H_{10}N_2$
- (*R*,*S*)-1,2-Propanediamine [10424-38-1]
  1,2-Diaminopropane (racemic)
  Group-member nr.: 31-009
- Trimethylhydrazine [1741-01-1]
  Group-member nr.: 34-005

$C_3H_{12}BN$
- Trimethylamineborane [75-22-9]
  N, *N*-Dimethylmethanamine compd. with borane (1:1)
  Group-member nr.: 72-006

C_3O_2
- 1,2-Propadiene-1,3-dione [504-64-3]
  Carbon suboxide
  Group-member nr.: 43-002

$C_4Br_2Cl_2F_6$
- 1,4-Dibromo-2,3-dichloro-1,1,2,3,4,4-hexafluorobutane [375-42-8]
  Group-member nr.: 25-026

C_4F_8
- Octafluorocyclobutane [115-25-3]
  Perfluorocyclobutane
  Group-member nr.: 21-007

$C_4H_2O_3$
- 2,5-Furandione [108-31-6]
  (*Z*)-Butenedioic acid anhydride
  Maleic anhydride
  Group-member nr.: 44-005

$C_4H_3Cl_3OS$
- *O*-Methyl ester 2,3,3-trichloro-2-propenethioic acid [76619-91-5]
  O-Methyl ester trichlorothioacrylic acid
  Methyl trichlorothioacrylate
  Group-member nr.: 64-007

$C_4H_4N_2$
- Butanedinitrile [110-61-2]
  Succinonitrile
  Ethylene dicyanide
  Group-member nr.: 32-006

C_4H_4O
- Furan [110-00-9]
  Furfuran
  Tetrol
  Group-member nr.: 46-006

$C_4H_4O_4$
- 1,4-Dioxane-2,5-dione [502-97-6]
  p-Dioxane-2,5-dione
  Glycolide
  Diglycolide
  Group-member nr.: 47-005

C_4H_4S
- Thiophene [110-02-1]
  Thiofuran
  Group-member nr.: 53-002

C_4H_5Cl
- 2-Chloro-1,3-butadiene [126-99-8]
  Chloroprene
  Group-member nr.: 22-027

$C_4H_5ClO_2$
- (*E*)-3-Chloro-2-butenoic acid [6214-28-4]
  trans-3-Chloro-2-butenoic acid
  3-Chlorocrotonic acid
  Group-member nr.: 61-014
- (*Z*)-3-Chloro-2-butenoic acid [6213-90-7]
  cis-3-Chloro-2-butenoic acid
  3-Chloroisocrotonic acid
  Group-member nr.: 61-015

$C_4H_5Cl_3O$
- 2,2,3-Trichlorobutanal [76-36-8]
  2,2,3-Trichlorobutyraldehyde
  Butylchloral
  Group-member nr.: 61-016

$C_4H_5Cl_3O_2$
- Ethyl trichloroacetate [515-84-4]
  Ethyl ester trichloroacetic acid
  Group-member nr.: 61-017

C_4H_5N
- Cyclopropanecarbonitrile [5500-21-0]
  Cyclopropyl cyanide
  Cyanocyclopropane
  Group-member nr.: 32-007
- 2-Methyl-2-propenenitrile [126-98-7]
  Methacrylonitrile
  Group-member nr.: 32-008
- 1*H*-Pyrrole [109-97-7]
  Azole
  Group-member nr.: 33-005

C_4H_5NO
- 4-Oxobutanenitrile [3515-93-3]
  β-Cyanopropionaldehyde
  Group-member nr.: 62-019

$C_4H_5NO_2$
- 2,5-Pyrrolidinedione [123-56-8]
  Succinimide
  Group-member nr.: 62-020

C_4H_5NS
- 3-Isothiocyanato-1-propene [57-06-7]
  Allyl isothiocyanate
  Group-member nr.: 64-008
- 2-Methylthiazole [3581-87-1]
  Group-member nr.: 64-009

C_4H_6
- 1,2-Butadiene [590-19-2]
  Group-member nr.: 13-003
- 1,3-Butadiene [106-99-0]
  Vinylethylene
  Divinyl
  Erythrene
  Group-member nr.: 13-004
- 1-Butyne [107-00-6]
  Ethylacetylene
  Group-member nr.: 13-005
- 2-Butyne [503-17-3]
  Dimethylacetylene
  Crotonylene
  Group-member nr.: 13-006

$C_4H_6Cl_2O_2$
- Ethyl dichloroacetate [535-15-9]
  Ethyl ester dichloroacetic acid
  Group-member nr.: 61-018

C_4H_6O
- 2-Butenal [4170-30-3]
  Crotonoaldehyde
  Group-member nr.: 43-005
- 2,3-Dihydrofuran [1191-99-7]
  Group-member nr.: 46-007

$C_4H_6O_2$
- (*E*)-2-Butenoic acid [107-93-7]
  trans-2-Butenoic acid
  Crotonic acid
  Group-member nr.: 44-006
- 2(3*H*)-Dihydrofuranone [96-48-0]
  β-Butyrolactone
  4-Butanolide
  Group-member nr.: 47-006
- Ethenyl acetate [108-05-4]
  Vinyl acetate
  Ethenyl ethanoate
  Group-member nr.: 45-005
- Methyl propenoate [96-33-3]
  Methyl acrylate
  Group-member nr.: 45-006
- 2-Methyl-2-propenoic acid [79-41-4]
  Methacrylic acid
  α-Methacrylic acid
  Group-member nr.: 44-007

$C_4H_6O_3$
- Acetic acid anhydride [108-24-7]
  Acetic anhydride
  Ethanoic acid anhydride
  Group-member nr.: 44-008
- 4-Methyl-1,3-dioxolan-2-one [108-32-7]
  Cyclic propylene ester carbonic acid
  Propylene carbonate
  Group-member nr.: 47-007

C_4H_7ClO
- Butanoyl chloride [141-75-3]
  Butyryl chloride
  Group-member nr.: 61-019
- 2-Methylpropanoyl chloride [79-30-1]
  2-Methylpropionyl chloride
  Isobutyryl chloride
  Group-member nr.: 61-020

$C_4H_7ClO_2$
- Ethyl chloroacetate [105-39-5]
  Ethyl ester chloroacetic acid
  Group-member nr.: 61-021

$C_4H_7Cl_2NSi$
- 3-(Dichloromethylsilyl)propanenitrile [1071-21-2]
  3-(Dichloromethylsilyl)propionitrile
  Dichloro-(2-cyanethyl)methylsilane
  Group-member nr.: 71-005

C_4H_7N
- Butanenitrile [109-74-0]
  Butyronitrile
  Propyl cyanide
  Group-member nr.: 32-009
- 2-Methylpropanenitrile [78-82-0]
  2-Methylpropionitrile
  Isobutyronitrile
  Isopropyl cyanide
  Group-member nr.: 32-010

C_4H_7NO
- 3-Methoxypropionitrile [110-67-8]
  Group-member nr.: 62-021
- 2-Pyrrolidinone [616-45-5]
  2-Pyrrolidone
  β-Butyrolactam
  Group-member nr.: 62-022

$C_4H_7NaO_2$
- Sodium salt butanoic acid [156-54-7]
  Sodium butanoate
  Natrium butyrate
  Group-member nr.: 74-003

C_4H_8
- 1-Butene [106-98-9]
  Group-member nr.: 13-007
- (*E*)-2-Butene [624-64-6]
  trans-2-Butene
  trans-Dimethylethylene
  Group-member nr.: 13-008
- (*Z*)-2-Butene [590-18-1]
  cis-2-Butene
  cis-Dimethylethylene
  Group-member nr.: 13-009
- Cyclobutane [287-23-0]
  Tetramethylene
  Group-member nr.: 12-002
- 2-Methyl-1-propene [115-11-7]
  Isobutene
  Group-member nr.: 13-010

$C_4H_8Cl_2$
- 1,4-Dichlorobutane [110-56-5]
  Tetramethylene dichloride
  Group-member nr.: 22-028

$C_4H_8Cl_2O$
- 1,1'-Oxybis(2-chloroethane) [111-44-4]
  Bis(2-chloroethyl) ether
  β,β'-Dichlorodiethyl ether
  Chlorex
  Group-member nr.: 61-022

C_4H_8O
- Butanal [123-72-8]
  Butyraldehyde
  Group-member nr.: 43-006
- 2-Butanone [78-93-3]
  Ethyl methyl ketone
  Group-member nr.: 43-007
- Ethyloxirane [106-88-7]
  1,2-Epoxybutane
  1,2-Butylene oxide
  Group-member nr.: 46-008
- 2-Methoxy-1-propene [116-11-0]
  Isopropenyl methyl ether
  Group-member nr.: 41-003
- Tetrahydrofuran [109-99-9]
  Oxolane
  Tetramethylene oxide
  Group-member nr.: 46-009

$C_4H_8O_2$
- Butanoic acid [107-92-6]
  Butyric acid
  Ethylacetic acid
  Propylformic acid
  Group-member nr.: 44-009
- 1,3-Dioxane [505-22-6]
  m-Dioxane
  Group-member nr.: 46-010
- 1,4-Dioxane [123-91-1]
  p-Dioxane
  1,4-Diethylene dioxide
  Dioxyethylene ether
  Diethylene ether
  Group-member nr.: 46-011
- Ethyl acetate [141-78-6]
  Ethyl ethanoate
  Group-member nr.: 45-007
- Methyl propanoate [554-12-1]
  Methyl propionate
  Group-member nr.: 45-008
- 2-Methylpropanoic acid [79-31-2]
  Isobutyric acid
  Group-member nr.: 44-010
- Propyl formate [110-74-7]
  Propyl methanoate
  Group-member nr.: 45-009

$C_4H_8O_2S$
- Tetrahydrothiophene 1,1-dioxide [126-33-0]
  Tetramethylene sulfone
  Sulfolane
  Group-member nr.: 63-004

$C_4H_8O_4$
- 1,3,5,7-Tetroxocane [293-30-1]
  1,3,5,7-Tetraoxacyclooctane
  Group-member nr.: 46-012

C_4H_8S
- Tetrahydrothiophene [110-01-0]
  Thiolane
  Tetramethylene sulfide
  Group-member nr.: 53-003

$C_4H_8S_2$
- 1,3-Dithiane [505-23-7]
  m-Dithiane
  Group-member nr.: 53-004
- 1,4-Dithiane [505-29-3]
  p-Dithiane
  Group-member nr.: 53-005

C_4H_9Br
- 1-Bromobutane [109-65-9]
  n-Butyl bromide
  Group-member nr.: 23-025
- 1-Bromo-2-methylpropane [78-77-3]
  Isobutyl bromide
  Group-member nr.: 23-026
- 2-Bromo-2-methylpropane [507-19-7]
  tert-Butyl bromide
  Group-member nr.: 23-027

C_4H_9Cl
- 1-Chlorobutane [109-69-3]
  n-Butyl chloride
  Group-member nr.: 22-029
- 1-Chloro-2-methylpropane [513-36-0]
  Isobutyl chloride
  Group-member nr.: 22-030
- 2-Chloro-2-methylpropane [507-20-0]
  tert-Butyl chloride
  Group-member nr.: 22-031

C_4H_9I
- 1-Iodo-2-methylpropane [513-38-2]
  Isobutyl iodide
  Group-member nr.: 24-005

C_4H_9N
- Pyrrolidine [123-75-1]
  Tetrahydropyrrole
  Azolidine
  Group-member nr.: 33-006

C_4H_9NO
- 2-Butanone oxime [96-29-7]
  Ethyl methyl ketoxime (unspecified stereoisomer)
  Group-member nr.: 62-023
- *N*, *N*-Dimethylacetamide [127-19-5]
  Group-member nr.: 62-024
- *N*-Ethylacetamide [625-50-3]
  N-Ethylethanamide
  Group-member nr.: 62-025

- *N*-Methylpropanamide [1187-58-2]
  N-Methylpropionamide
  Group-member nr.: 62-026
- Morpholine [110-91-8]
  Tetrahydro-4*H*-1,4-oxazine
  Diethylenimide oxide
  Group-member nr.: 62-027

C_4H_{10}
- Butane [106-97-8]
  Group-member nr.: 11-006
- 2-Methylpropane [75-28-5]
  Isobutane
  Trimethylmethane
  Group-member nr.: 11-007

$C_4H_{10}Cl_2Si$
- Dichlordiethylsilane [1719-53-5]
  Group-member nr.: 71-006

$C_4H_{10}Hg$
- Diethylmercury [627-44-1]
  Group-member nr.: 73-008

$C_4H_{10}N_2$
- Piperazine [110-85-0]
  Hexahydropyrazine
  Perhydro-1,4-diazine
  Diethylenediamine
  Group-member nr.: 33-007

$C_4H_{10}O$
- 1-Butanol [71-36-3]
  Butyl alcohol
  Group-member nr.: 42-013
- 2-Butanol [78-92-2]
  sec-Butyl alcohol
  Methyl ethyl carbinol (unspecified chirality)
  Group-member nr.: 42-014
- (*R,S*)-2-Butanol [15892-23-6]
  sec-Butyl alcohol
  Methyl ethyl carbinol (racemic)
  Group-member nr.: 42-015
- (*S*)-2-Butanol [4221-99-2]
  D-*sec*-Butyl alcohol
  D-Methyl ethyl carbinol
  Group-member nr.: 42-016
- 1-Methoxypropane [557-17-5]
  Methyl propyl ether
  Group-member nr.: 41-004
- 2-Methoxypropane [598-53-8]
  Methyl 1-methylethyl ether
  Isopropyl methyl ether
  Group-member nr.: 41-005
- 2-Methyl-1-propanol [78-83-1]
  Isobutyl alcohol
  Group-member nr.: 42-017
- 2-Methyl-2-propanol [75-65-0]
  tert-Butyl alcohol
  Trimethyl carbinol
  Group-member nr.: 42-018
- 1,1'-Oxybisethane [60-29-7]
  Diethyl ether
  Ethyl ether
  Ethyl oxide
  Diethyl oxide
  Group-member nr.: 41-006

$C_4H_{10}O_2$
- 1,3-Butanediol [107-88-0]
  1,3-Butylene glycol
  Group-member nr.: 42-019
- 1,4-Butanediol [110-63-4]
  1,4-Butylene glycol
  Tetramethylene glycol
  Group-member nr.: 42-020
- 2,3-Butanediol [513-85-9]
  2,3-Butylene glycol
  Group-member nr.: 42-021
- 1,2-Dimethoxyethane [110-71-4]
  2,5-Dioxahexane
  Ethylene glycol dimethyl ether
  Monoglyme
  GDME
  Group-member nr.: 41-007
- 2-Ethoxyethanol [110-80-5]
  3-Oxa-1-pentanol
  Ethyl cellosolve
  Ethylene glycol monoethyl ether
  Group-member nr.: 47-008

$C_4H_{10}O_2Se$
- 2,2'-Selenodiethanol [27974-49-8]
  β-Selenium diglycol
  Group-member nr.: 73-009

$C_4H_{10}O_3$
- 2,2'-Oxybisethanol [111-46-6]
  1,5-Dihydroxy-3-oxapentane
  2,2'-Dihydroxydiethyl ether
  Diethylene glycol
  Group-member nr.: 47-009

$C_4H_{10}O_4$
- (*R**, *S**)-1,2,3,4-Butanetetrol [149-32-6]
  Erythro-1,2,3,4-butanetetrol
  Erythritol
  Group-member nr.: 42-022

$C_4H_{10}S$
- 1-Butanethiol [109-79-5]
  1-Butyl mercaptan
  Group-member nr.: 52-005
- 2-Butanethiol [513-53-1]
  2-Butyl mercaptan
  sec-Butyl mercaptan
  Group-member nr.: 52-006

- 2-Methyl-1-propanethiol [513-44-0]
  Isobutyl mercaptan
  Group-member nr.: 52-007
- 2-Methyl-2-propanethiol [75-66-1]
  tert-Butyl mercaptan
  Group-member nr.: 52-008
- 1-(Methylthio)propane [3877-15-4]
  Methyl propyl sulfide
  Group-member nr.: 51-004
- 2-(Methylthio)propane [1551-21-9]
  Methyl 1-methylethyl sulfide
  Isopropyl methyl sulfide
  Group-member nr.: 51-005
- 1,1'-Thiobisethane [352-93-2]
  Diethyl sulfide
  Group-member nr.: 51-006

$C_4H_{10}S_2$
- 3,4-Dithiahexane [110-81-6]
  Diethyl disulfide
  Ethyl disulfide
  Group-member nr.: 51-007

$C_4H_{10}Zn$
- Diethylzinc [557-20-0]
  Group-member nr.: 73-010

$C_4H_{11}N$
- 1-Butanamine [109-73-9]
  n-Butylamine
  Group-member nr.: 31-010
- *N*-Ethylethanamine [109-89-7]
  Diethylamine
  Group-member nr.: 31-011
- 2-Methyl-1-propanamine [78-81-9]
  Isobutylamine
  Group-member nr.: 31-012
- 2-Methyl-2-propanamine [75-64-9]
  tert-Butylamine
  Group-member nr.: 31-013

$C_4H_{11}NO$
- 2-Amino-2-methyl-1-propanol [124-68-5]
  Isobutanolamine
  Group-member nr.: 62-028
- *N*, *N*-Diethylhydroxylamine [3710-84-7]
  Group-member nr.: 62-029
- 3-Methoxy-1-propanamine [5332-73-0]
  3-Methoxypropylamine
  4-Oxapentanamine
  Group-member nr.: 62-030

$C_4H_{11}NO_2$
- 2-Amino-2-methyl-1,3-propanediol [115-69-5]
  Group-member nr.: 62-031

$C_4H_{11}NO_3$
- 2-Amino-2-(hydroxymethyl)-1,3-propanediol [77-86-1]
  Trometamol
  Group-member nr.: 62-032

$C_4H_{12}CdSe$
- Dimethyl[selenobis(methane)]cadmium [143481-65-6]
  Group-member nr.: 73-011

$C_4H_{12}CdTe$
- Dimethyl[tellurobis(methane)]cadmium [143481-66-7]
  Group-member nr.: 73-012

$C_4H_{12}Ge$
- Tetramethylgermane [865-52-1]
  Group-member nr.: 73-013

$C_4H_{12}N_2$
- 2-Methyl-1,2-propanediamine [811-93-8]
  1,2-Diamino-2-methylpropane
  Group-member nr.: 31-014

$C_4H_{12}O_4Si$
- Tetramethyl ester silicic acid [681-84-5]
  Tetramethyl orthosilicate
  Tetramethoxysilane
  Group-member nr.: 71-007

$C_4H_{12}Pb$
- Tetramethylplumbane [75-74-1]
  Tetramethyllead
  Group-member nr.: 73-014

$C_4H_{12}SeZn$
- Dimethyl[selenobis(methane)]zinc [108430-95-1]
  Complex dimethylzinc with dimethylselenium
  Group-member nr.: 73-015

$C_4H_{12}Si$
- Tetramethylsilane [75-76-3]
  Group-member nr.: 71-008

$C_4H_{12}Sn$
- Tetramethylstannane [594-27-4]
  Tetramethyltin
  Group-member nr.: 73-016

$C_4H_{12}TeZn$
- Dimethyl[tellurobis(methane)]zinc [127283-03-8]
  Complex dimethylzinc with dimethyltellurium
  Group-member nr.: 73-017

$C_4H_{13}N_3$
- *N*-(2-Aminoethyl)-1,2-ethanediamine [111-40-0]
  Diethylenetriamine
  Group-member nr.: 31-015

C_4NiO_4
- Nickel carbonyl [13463-39-3]
  Group-member nr.: 02-029

$C_5F_{11}N$
- Undecafluoropiperidine [836-77-1]
  Perfluoropiperidine
  Group-member nr.: 64-010

C_5F_{12}
- Dodecafluoropentane [678-26-2]
  Perfluoropentane
  Group-member nr.: 21-008

$C_5F_{13}N$
- 1,1,2,2,2-Pentafluoro-*N*-(pentafluoroethyl)-*N*-(trifluoromethyl)-ethanamine [758-48-5]
  Group-member nr.: 64-011

$C_5H_3F_7O_2$
- Methyl heptafluorobutanoate [356-24-1]
  Methyl ester heptafluorobutanoic acid
  Methyl perfluorobutyrate
  Group-member nr.: 61-023

$C_5H_4O_2$
- 2-Furancarboxaldehyde [98-01-1]
  Furfural
  Pyromucic aldehyde
  Furfuraldehyde
  Group-member nr.: 47-010

$C_5H_5Cl_3O_2$
- 2-Propenyl trichloroacetate [6304-34-3]
  2-Propenyl ester trichloroacetic acid
  Allyl trichloroacetate
  Group-member nr.: 61-024

C_5H_5N
- Bicyclo[1.1.0]butane-1-carbonitrile [16955-35-4]
  1-Bicyclobutyl cyanide
  1-Cyanobicyclobutane
  Group-member nr.: 32-011
- Pyridine [110-86-1]
  Azine
  Group-member nr.: 33-008

$C_5H_6Cl_2O_2$
- 2-Propenyl dichloroacetate [30895-77-3]
  2-Propenyl ester dichloroacetic acid
  Allyl dichloroacetate
  Group-member nr.: 61-025

$C_5H_6N_2$
- Dimethylpropanedinitrile [7321-55-3]
  2,2-Dicyanopropane
  Dimethylmalononitrile
  Group-member nr.: 32-012
- Pentanedinitrile [544-13-8]
  1,3-Dicyanopropane
  Glutaronitrile
  Trimethylenedicyanide
  Group-member nr.: 32-013

C_5H_6O
- 2-Methylfuran [534-22-5]
  Sylvan
  Group-member nr.: 46-013

$C_5H_6O_2$
- 2-Furanmethanol [98-00-0]
  Furfuryl alcohol
  Furyl carbinol
  Group-member nr.: 47-011

C_5H_6S
- 2-Methylthiophene [554-14-3]
  Group-member nr.: 53-006
- 3-Methylthiophene [616-44-4]
  Group-member nr.: 53-007

$C_5H_7ClO_2$
- 2-Propenyl chloroacetate [2916-14-5]
  2-Propenyl ester chloroacetic acid
  Allyl chloroacetate
  Group-member nr.: 61-026

$C_5H_7Cl_3O_2$
- Propyl trichloroacetate [13313-91-2]
  Propyl ester trichloroacetic acid
  Group-member nr.: 61-027

C_5H_7N
- Cyclobutanecarbonitrile [4426-11-3]
  Cyclobutyl cyanide
  Cyanocyclobutane
  Group-member nr.: 32-014
- 1-Methyl-1*H*-pyrrole [96-54-8]
  Group-member nr.: 33-009

$C_5H_7NO_2$
- Ethyl ester cyanoacetic acid [105-56-6]
  Ethyl cyanoacetate
  Group-member nr.: 62-033

C_5H_8
- Cyclopentene [142-29-0]
  Group-member nr.: 14-001
- 2-Methyl-1,3-butadiene [78-79-5]
  Isoprene
  Group-member nr.: 13-011
- 3-Methyl-1,2-butadiene [598-25-4]
  Group-member nr.: 13-012
- Methylenecyclobutane [1120-56-5]
  Group-member nr.: 12-003
- 1,2-Pentadiene [591-95-7]
  Group-member nr.: 13-013
- (*E*)-1,3-Pentadiene [2004-70-8]
  trans-1,3-Pentadiene
  Group-member nr.: 13-014
- (*Z*)-1,3-Pentadiene [1574-41-0]
  cis-1,3-Pentadiene
  Group-member nr.: 13-015
- 1,4-Pentadiene [591-93-5]
  Group-member nr.: 13-016
- 2,3-Pentadiene [591-96-8]
  Group-member nr.: 13-017
- Spiropentane [157-40-4]
  Spirocyclane
  Cyclopropanespirocyclopropane
  Group-member nr.: 12-004

$C_5H_8Br_4$
- 1,3-Dibromo-2,2-bis(bromomethyl)propane [3229-00-3]
  2,2-Bis(bromomethyl)-1,3-dibromopropane
  Pentaerythrityl tetrabromide
  Group-member nr.: 23-028

$C_5H_8Cl_2O$
- 3,3-Bis(chloromethyl)oxetane [78-71-7]
  3,3-Bis(chloromethyl)oxacyclobutane
  Group-member nr.: 61-028

$C_5H_8Cl_2O_2$
- Ethyl 2,3-dichloropropanoate [6628-21-3]
  Ethyl ester 2,3-dichloropropanoic acid
  Group-member nr.: 61-029
- Propyl dichloroacetate [37587-81-8]
  Propyl ester dichloroacetic acid
  Group-member nr.: 61-030

$C_5H_8Cl_4$
- 1,3-Dichloro-2,2-bis(chloromethyl)propane [3228-99-7]
  2,2-Bis(chloromethyl)-1,3-dichloropropane
  Pentaerythrityl tetrachloride
  Group-member nr.: 22-032

$C_5H_8F_4$
- 1,3-Difluoro-2,2-bis(fluoromethyl)propane [338-23-8]
  2,2-Bis(fluoromethyl)-1,3-difluoropropane
  Pentaerythrityl tetrafluoride
  Group-member nr.: 21-009

C_5H_8O
- Cyclopentanone [120-92-3]
  Group-member nr.: 43-008

$C_5H_8O_2$
- Methyl 2-methyl-2-propenoate [80-62-6]
  Methyl methacrylate
  Group-member nr.: 45-010
- 2,4-Pentanedione [123-54-6]
  Acetylacetone
  Diacetylmethane
  Group-member nr.: 43-009
- 2-Propenyl acetate [591-87-7]
  2-Propenyl ethanoate
  Allyl acetate
  Group-member nr.: 45-011
- Tetrahydro-2*H*-pyran-2-one [542-28-9]
  δ-Valerolactone
  5-Pentanolide
  Group-member nr.: 47-012

C_5H_9ClO
- Pentanoyl chloride [638-29-9]
  Valeryl chloride
  Group-member nr.: 61-031

$C_5H_9ClO_2$
- Ethyl 2-chloropropanoate [535-13-7]
  Ethyl ester 2-chloropropanoic acid
  Ethyl α-chloropropionate
  Group-member nr.: 61-032
- Propyl chloroacetate [5396-24-7]
  Propyl ester chloroacetic acid
  Group-member nr.: 61-033

C_5H_9N
- 2,2-Dimethylpropanenitrile [630-18-2]
  2-Cyano-2-methylpropane
  Pivalonitrile
  Trimethylacetonitrile
  Group-member nr.: 32-015
- Pentanenitrile [110-59-8]
  Valeronitrile
  Butyl cyanide
  Group-member nr.: 32-016

C_5H_9NO
- 1-Methyl-2-pyrrolidinone [872-50-4]
  1-Methyl-2-pyrrolidone
  Group-member nr.: 62-034
- 2-Piperidinone [675-20-7]
  δ-Valerolactam
  2-Piperidone
  Group-member nr.: 62-035

C_5H_{10}
- Cyclopentane [287-92-3]
  Pentamethylene
  Group-member nr.: 12-005
- 2-Methyl-1-butene [563-46-2]
  Group-member nr.: 13-018
- 2-Methyl-2-butene [513-35-9]
  Trimethylethylene
  β-Isoamylene
  Group-member nr.: 13-019
- 3-Methyl-1-butene [563-45-1]
  Isopropylethylene
  α-Isoamylene
  Group-member nr.: 13-020
- 1-Pentene [109-67-1]
  Group-member nr.: 13-021
- 2-Pentene [109-68-2]
  β-Amylene
  Methylethylethylene (unspecified stereoisomer)
  Group-member nr.: 13-022
- (*E*)-2-Pentene [646-04-8]
  trans-2-Pentene
  trans-β-Amylene
  trans-Methylethylethylene
  Group-member nr.: 13-023
- (*Z*)-2-Pentene [627-20-3]
  cis-2-Pentene
  cis-β-Amylene
  cis-Methylethylethylene
  Group-member nr.: 13-024

$C_5H_{10}Cl_2$
- 1,5-Dichloropentane [628-76-2]
  Pentamethylene dichloride
  Group-member nr.: 22-033

$C_5H_{10}N_2$
- 3-(Dimethylamino)propanenitrile [1738-25-6]
  3-(Dimethylamino)propionitrile
  Group-member nr.: 34-006

$C_5H_{10}O$
- Cyclopentanol [96-41-3]
  Cyclopentyl alcohol
  Group-member nr.: 42-023

- 2,2-Dimethylpropanal [630-19-3]
  Pivalaldehyde
  Trimethylacetaldehyde
  Group-member nr.: 43-010
- 3-Methyl-2-butanone [563-80-4]
  Isopropyl methyl ketone
  Group-member nr.: 43-011
- 2-Methyl-3-buten-2-ol [115-18-4]
  Group-member nr.: 42-024
- Pentanal [110-62-3]
  Valeraldehyde
  Pentyl aldehyde
  Amyl aldehyde
  Group-member nr.: 43-012
- 2-Pentanone [107-87-9]
  Methyl propyl ketone
  Group-member nr.: 43-013
- 3-Pentanone [96-22-0]
  Diethyl ketone
  Metacetone
  Ethyl propionyl
  Propione
  Group-member nr.: 43-014
- Tetrahydropyran [142-68-7]
  Oxane
  Pentamethylene oxide
  Group-member nr.: 46-014

$C_5H_{10}O_2$
- Butyl formate [592-84-7]
  Butyl methanoate
  Group-member nr.: 45-012
- 1,3-Dioxepane [505-65-7]
  m-Dioxepane
  Group-member nr.: 46-015
- Ethyl propanoate [105-37-3]
  Ethyl propionate
  Group-member nr.: 45-013
- Methyl butanoate [623-42-7]
  Methyl butyrate
  Group-member nr.: 45-014
- 3-Methylbutanoic acid [503-74-2]
  Isovaleric acid
  Group-member nr.: 44-011
- 1-Methylethyl acetate [108-21-4]
  Isopropyl acetate
  1-Methylethyl ethanoate
  Group-member nr.: 45-016
- Methyl 2-methylpropanoate [547-63-7]
  Methyl isobutyrate
  Group-member nr.: 45-015
- 2-Methylpropyl formate [542-55-2]
  2-Methylpropyl methanoate
  Isobutyl formate
  Group-member nr.: 45-017
- Pentanoic acid [109-52-4]
  Valeric acid
  Group-member nr.: 44-012
- Propyl acetate [109-60-4]
  Propyl ethanoate
  Group-member nr.: 45-018
- Tetrahydro-2-furanmethanol [97-99-4]
  Tetrahydrofurfuryl alcohol
  Group-member nr.: 47-013

$C_5H_{10}O_3$
- Diethyl carbonate [105-58-8]
  Ethyl carbonate
  Group-member nr.: 45-019
- 2-Methoxyethanol acetate [110-49-6]
  2-Methoxyethyl acetate
  Group-member nr.: 47-014

$C_5H_{10}O_5$
- 1,3,5,7,9-Pentoxecane [16528-92-0]
  Pentoxane
  Group-member nr.: 46-016

$C_5H_{10}S$
- Cyclopentanethiol [1679-07-8]
  Cyclopentyl mercaptan
  Group-member nr.: 52-009
- 2-Methyltetrahydrothiophene [1795-09-1]
  2-Methylthiolane
  2-Methylcyclothiapentane
  Group-member nr.: 53-008
- 3-Methyltetrahydrothiophene [4740-00-5]
  3-Methylthiolane
  3-Methylcyclothiapentane
  Group-member nr.: 53-009
- Tetrahydro-2*H*-thiopyran [1613-51-0]
  Thiacyclohexane
  Pentamethylene sulfide
  Group-member nr.: 53-010

$C_5H_{11}Br$
- 1-Bromo-3-methylbutane [107-82-4]
  Isoamyl bromide
  Group-member nr.: 23-029
- 1-Bromopentane [110-53-2]
  n-Amyl bromide
  Group-member nr.: 23-030

$C_5H_{11}Cl$
- 1-Chloro-3-methylbutane [107-84-6]
  Isoamyl chloride
  Group-member nr.: 22-034

$C_5H_{11}I$
- 1-Iodo-3-methylbutane [541-28-6]
  Isoamyl iodide
  Group-member nr.: 24-006

$C_5H_{11}N$
- Cyclopentanamine [1003-03-8]
  Cyclopentylamine
  Group-member nr.: 31-016

- 1-Methylpyrrolidine [120-94-5]
  N-Methylpyrrolidine
  Group-member nr.: 33-010
- 3-Methylpyrrolidine [34375-89-8]
  Group-member nr.: 33-011
- Piperidine [110-89-4]
  Pentamethylenimine
  Hexahydropyridine
  Perhydroazine
  Group-member nr.: 33-012

$C_5H_{11}NO$
- *N*,2-Dimethylpropanamide [2675-88-9]
  N-Methylisobutyramide
  Group-member nr.: 62-036
- *N*-Methylbutanamide [17794-44-4]
  N-Methylbutyramide
  Group-member nr.: 62-037
- *N*-(1-Methylethyl)acetamide [1118-69-0]
  N-(1-Methylethyl)ethanamide
  N-Isopropylacetamide
  Group-member nr.: 62-038
- *N*-Propylacetamide [5331-48-6]
  N-Propylethanamide
  Group-member nr.: 62-039

C_5H_{12}
- 2,2-Dimethylpropane [463-82-1]
  Neopentane
  Tetramethylmethane
  Group-member nr.: 11-008
- 2-Methylbutane [78-78-4]
  Isopentane
  Group-member nr.: 11-009
- Pentane [109-66-0]
  Group-member nr.: 11-010

$C_5H_{12}N_2O$
- Tetramethylurea [632-22-4]
  Group-member nr.: 62-040

$C_5H_{12}O$
- 1-Ethoxypropane [628-32-0]
  Ethyl propyl ether
  Group-member nr.: 41-008
- 1-Methoxybutane [628-28-4]
  Butyl methyl ether
  Group-member nr.: 41-009
- 2-Methoxy-2-methylpropane [1634-04-4]
  1,1-Dimethylethyl methyl ether
  tert-Butyl methyl ether
  Group-member nr.: 41-010
- 2-Methyl-1-butanol [137-32-6]
  sec-Butyl carbinol
  Group-member nr.: 42-025
- 2-Methyl-2-butanol [75-85-4]
  tert-Amyl alcohol
  tert-Pentyl alcohol
  Dimethyl ethyl carbinol
  Group-member nr.: 42-026
- 3-Methyl-1-butanol [123-51-3]
  Isopentyl alcohol
  Isoamyl alcohol
  Group-member nr.: 42-027
- 3-Methyl-2-butanol [598-75-4]
  sec-Isoamyl alcohol
  Group-member nr.: 42-028
- 1-Pentanol [71-41-0]
  n-Amyl alcohol
  Group-member nr.: 42-029
- 2-Pentanol [6032-29-7]
  sec-Amyl alcohol
  Methyl propyl carbinol
  Group-member nr.: 42-030
- 3-Pentanol [584-02-1]
  1-Ethyl-1-propanol
  Diethyl carbinol
  Group-member nr.: 42-031

$C_5H_{12}O_2$
- 2,2-Dimethoxypropane [77-76-9]
  Acetone dimethyl acetal
  Group-member nr.: 41-011
- 2,2-Dimethyl-1,3-propanediol [126-30-7]
  Group-member nr.: 42-032
- 1-Ethoxy-2-methoxyethane [5137-45-1]
  2,5-Dioxaheptane
  Ethylene glycol ethyl ether methyl ether
  Group-member nr.: 41-012
- 2-(1-Methylethoxy)ethanol [109-59-1]
  4-Methyl-3-oxa-1-pentanol
  2-Isopropoxyethanol
  Ethylene glycol monoisopropyl ether
  Group-member nr.: 47-015
- 1,5-Pentanediol [111-29-5]
  Group-member nr.: 42-033
- 2-Propoxyethanol [2807-30-9]
  3-Oxa-1-hexanol
  Ethylene glycol monopropyl ether
  Propyl cellosolve
  Group-member nr.: 47-016

$C_5H_{12}O_3$
- 2-(2-Methoxyethoxy)ethanol [111-77-3]
  Diethylene glycol monomethyl ether
  Group-member nr.: 47-017

$C_5H_{12}S$
- 1-(Ethylthio)propane [4110-50-3]
  Ethyl propyl sulfide
  Group-member nr.: 51-008
- 2-Methyl-2-butanethiol [1679-09-0]
  2-Methyl-2-butyl mercaptan
  tert-Amyl mercaptan
  Group-member nr.: 52-010
- 3-Methyl-1-butanethiol [541-31-1]
  3-Methylbutyl mercaptan
  Isopentyl mercaptan
  Isoamyl mercaptan
  Group-member nr.: 52-011

- 3-Methyl-2-butanethiol [2084-18-6]
  3-Methyl-2-butyl mercaptan
  sec-Isoamyl mercaptan
  Group-member nr.: 52-012
- 2-Methyl-2-(methylthio)propane [6163-64-0]
  1,1-Dimethylethyl methyl sulfide
  tert-Butyl methyl sulfide
  Group-member nr.: 51-009
- 1-(Methylthio)butane [628-29-5]
  Butyl methyl sulfide
  Group-member nr.: 51-010
- 2-(Methylthio)butane [10359-64-5]
  3-Methyl-2-thiapentane
  Methyl 1-methylpropyl sulfide
  sec-Butyl methyl sulfide
  Group-member nr.: 51-011
- 1-Pentanethiol [110-66-7]
  1-Pentyl mercaptan
  Group-member nr.: 52-013
- Tetrakis(methylthia)methane [6156-25-8]
  Tetramethyl ester tetrathiacarbonic acid
  Group-member nr.: 51-012

$C_5H_{12}Si$
- 1,1-Dimethylsilacyclobutane [2295-12-7]
  Group-member nr.: 71-009
- Ethenyltrimethylsilane [754-05-2]
  Trimethylvinylsilane
  Group-member nr.: 71-010

$C_5H_{13}N$
- *N*-Ethyl-*N*-methylethanamine [616-39-7]
  N-Methyldiethylamine
  N, *N*-Diethylmethylamine
  Group-member nr.: 31-017
- 1-Pentanamine [110-58-7]
  Pentylamine
  n-Amylamine
  Group-member nr.: 31-018

$C_5H_{13}NO$
- 2-(Ethylmethylamino)ethanol [2893-43-8]
  N, *N*-Ethylmethylethanolamine
  Group-member nr.: 62-041

$C_5H_{14}N_2$
- *N*, *N*-Dimethyl-1,3-propanediamine [109-55-7]
  N, *N*-Dimethylpropylenediamine
  Group-member nr.: 31-019

C_6BrF_5
- Bromopentafluorobenzene [344-04-7]
  Group-member nr.: 25-027

$C_6Br_2Cl_3F_9$
- 1,6-Dibromo-2,3,5-trichloro-1,1,2,3,4,4,5,6,6-nonafluorohexane [85131-86-8]
  Group-member nr.: 25-028

C_6ClF_5
- Chloropentafluorobenzene [344-07-0]
  Group-member nr.: 25-029

$C_6Cl_3F_3$
- 1,3,5-Trichloro-2,4,6-trifluorobenzene [319-88-0]
  Group-member nr.: 25-030

C_6D_6
- Benzene-d_6 [1076-43-3]
  Hexadeuterobenzene
  Group-member nr.: 14-002

C_6D_{12}
- Cyclohexane-d_{12} [1735-17-7]
  Dodecadeuterocyclohexane
  Group-member nr.: 12-006

$C_6F_5NO_2$
- Pentafluoronitrobenzene [880-78-4]
  Group-member nr.: 64-012

C_6F_6
- Hexafluorobenzene [392-56-3]
  Perfluorobenzene
  Group-member nr.: 21-010

C_6F_{14}
- Tetradecafluorohexane [355-42-0]
  Perfluorohexane
  Group-member nr.: 21-011

$C_6F_{15}N$
- 1,1,2,2,2-Pentafluoro-*N*, *N*-bis(pentafluoroethyl)-ethanamine [359-70-6]
  Group-member nr.: 64-013

C_6HF_5
- Pentafluorobenzene [363-72-4]
  Group-member nr.: 21-012

C_6HF_5O
- Pentafluorophenol [771-61-9]
  Group-member nr.: 61-034

$C_6H_2F_4$
- 1,2,3,4-Tetrafluorobenzene [551-62-2]
  Group-member nr.: 21-013
- 1,2,3,5-Tetrafluorobenzene [2367-82-0]
  Group-member nr.: 21-014
- 1,2,4,5-Tetrafluorobenzene [327-54-8]
  Group-member nr.: 21-015

$C_6H_2F_5N$
- 2,3,4,5,6-Pentafluorobenzenamine [771-60-8]
  Pentafluoroaniline
  Group-member nr.: 64-014

$C_6H_3Cl_3$
- 1,2,4-Trichlorobenzene [120-82-1]
  Group-member nr.: 22-035

$C_6H_3Cl_4N$
- 2-Chloro-6-(trichloromethyl)pyridine [1929-82-4]
  Group-member nr.: 64-015

C_6H_4BrCl
- 1-Bromo-2-chlorobenzene [694-80-4]
  o-Bromochlorobenzene
  Group-member nr.: 25-031
- 1-Bromo-3-chlorobenzene [108-37-2]
  m-Bromochlorobenzene
  Group-member nr.: 25-032
- 1-Bromo-4-chlorobenzene [106-39-8]
  p-Bromochlorobenzene
  Group-member nr.: 25-033

C_6H_4BrI
- 1-Bromo-2-iodobenzene [583-55-1]
  o-Bromoiodobenzene
  Group-member nr.: 25-034
- 1-Bromo-3-iodobenzene [591-18-4]
  m-Bromoiodobenzene
  Group-member nr.: 25-035

$C_6H_4BrNO_2$
- 1-Bromo-3-nitrobenzene [585-79-5]
  m-Bromonitrobenzene
  Group-member nr.: 64-016

$C_6H_4Br_2$
- 1,2-Dibromobenzene [583-53-9]
  o-Dibromobenzene
  Group-member nr.: 23-031
- 1,3-Dibromobenzene [108-36-1]
  m-Dibromobenzene
  Group-member nr.: 23-032

$C_6H_4Br_2O$
- 2,4-Dibromophenol [615-58-7]
  Group-member nr.: 61-035

$C_6H_4ClNO_2$
- 1-Chloro-3-nitrobenzene [121-73-3]
  m-Chloronitrobenzene
  Group-member nr.: 64-017
- 1-Chloro-4-nitrobenzene [100-00-5]
  p-Chloronitrobenzene
  Group-member nr.: 64-018

$C_6H_4Cl_2$
- 1,2-Dichlorobenzene [95-50-1]
  o-Dichlorobenzene
  Group-member nr.: 22-036
- 1,3-Dichlorobenzene [541-73-1]
  m-Dichlorobenzene
  Group-member nr.: 22-037
- 1,4-Dichlorobenzene [106-46-7]
  p-Dichlorobenzene
  Group-member nr.: 22-038

$C_6H_4F_2$
- 1,2-Difluorobenzene [367-11-3]
  o-Difluorobenzene
  Group-member nr.: 21-016
- 1,3-Difluorobenzene [372-18-9]
  m-Difluorobenzene
  Group-member nr.: 21-017
- 1,4-Difluorobenzene [540-36-3]
  p-Difluorobenzene
  Group-member nr.: 21-018

$C_6H_4I_2$
- 1,2-Diiodobenzene [615-42-9]
  o-Diiodobenzene
  Group-member nr.: 24-007
- 1,3-Diiodobenzene [626-00-6]
  m-Diiodobenzene
  Group-member nr.: 24-008

$C_6H_4N_2O_4$
- 1,2-Dinitrobenzene [528-29-0]
  o-Dinitrobenzene
  Group-member nr.: 62-042
- 1,3-Dinitrobenzene [99-65-0]
  m-Dinitrobenzene
  Group-member nr.: 62-043
- 1,4-Dinitrobenzene [100-25-4]
  p-Dinitrobenzene
  Group-member nr.: 62-044

$C_6H_4O_2$
- 2,5-Cyclohexadiene-1,4-dione [106-51-4]
  p-Benzoquinone
  p-Quinone
  Group-member nr.: 43-015

C_6H_5Br
- Bromobenzene [108-86-1]
  Phenyl bromide
  Group-member nr.: 23-033

C_6H_5BrO
- 4-Bromophenol [106-41-2]
  p-Bromophenol
  Group-member nr.: 61-036

C_6H_5Cl
- Chlorobenzene [108-90-7]
  Phenyl chloride
  Group-member nr.: 22-039

C_6H_5ClO
- 2-Chlorophenol [95-57-8]
  o-Chlorophenol
  Group-member nr.: 61-037

$C_6H_5Cl_3Si$
- Trichlorophenylsilane [98-13-5]
  Group-member nr.: 71-011

C_6H_5F
- Fluorobenzene [462-06-6]
  Group-member nr.: 21-019

C_6H_5FO
- 4-Fluorophenol [371-41-5]
  p-Fluorophenol
  Group-member nr.: 61-038

C_6H_5I
- Iodobenzene [591-50-4]
  Group-member nr.: 24-009

$C_6H_5NO_2$
- Nitrobenzene [98-95-3]
  Group-member nr.: 62-045

$C_6H_5NO_3$
- 2-Nitrophenol [88-75-5]
  o-Nitrophenol
  Group-member nr.: 62-046
- 3-Nitrophenol [554-84-7]
  m-Nitrophenol
  Group-member nr.: 62-047
- 4-Nitrophenol [100-02-7]
  p-Nitrophenol
  Group-member nr.: 62-048

C_6H_6
- Benzene [71-43-2]
  Group-member nr.: 14-003

C_6H_6ClN
- 3-Chlorobenzenamine [108-42-9]
  m-Chloroaniline
  Group-member nr.: 64-019

C_6H_6FN
- 4-Fluorobenzenamine [371-40-4]
  p-Fluoroaniline
  Group-member nr.: 64-020

$C_6H_6N_2O_2$
- 2-Nitrobenzenamine [88-74-4]
  o-Nitroaniline
  Group-member nr.: 62-049
- 3-Nitrobenzenamine [99-09-2]
  m-Nitroaniline
  Group-member nr.: 62-050
- 4-Nitrobenzenamine [100-01-6]
  p-Nitroaniline
  Group-member nr.: 62-051

C_6H_6O
- Phenol [108-95-2]
  Group-member nr.: 42-034

$C_6H_6O_2$
- 1,2-Benzenediol [120-80-9]
  1,2-Dihydroxybenzene
  Pyrocatechol
  Catechol
  Group-member nr.: 42-035
- 1,3-Benzenediol [108-46-3]
  1,3-Dihydroxybenzene
  Resorcinol
  Group-member nr.: 42-036
- 1,4-Benzenediol [123-31-9]
  1,4-Dihydroxybenzene
  Hydroquinone
  Group-member nr.: 42-037

C_6H_6S
- Benzenethiol [108-98-5]
  Thiophenol
  Phenyl mercaptan
  Group-member nr.: 52-014

C_6H_7N
- Benzenamine [62-53-3]
  Aniline
  Aminobenzene
  Phenylamine
  Group-member nr.: 31-020
- Bicyclo[2.1.0]pentane-1-carbonitrile [31357-71-8]
  1-Bicyclo[2.1.0]pentyl cyanide
  1-Cyanobicyclo[2.1.0]pentane
  Group-member nr.: 32-017
- 3-Methylenecyclobutanecarbonitrile [15760-35-7]
  3-Methylenecyclobutyl cyanide
  1-Cyano-3-methylenecyclobutane
  Group-member nr.: 32-018
- 2-Methylpyridine [109-06-8]
  α-Picoline
  Group-member nr.: 33-013
- 3-Methylpyridine [108-99-6]
  β-Picoline
  Group-member nr.: 33-014
- 4-Methylpyridine [108-89-4]
  γ-Picoline
  Group-member nr.: 33-015

C_6H_8
- 1,3-Cyclohexadiene [592-57-4]
  Group-member nr.: 14-004
- 1,4-Cyclohexadiene [628-41-1]
  Group-member nr.: 14-005

$C_6H_8N_2$
- 1,3-Benzenediamine [108-45-2]
  1,3-Phenylenediamine
  Group-member nr.: 31-021
- Phenylhydrazine [100-63-0]
  Group-member nr.: 34-007

$C_6H_8O_2$
- 1,4-Cyclohexanedione [637-88-7]
  Tetrahydroquinone
  Group-member nr.: 43-016
- Methyl bicyclo[1.1.0]butane-1-carboxylate [4935-01-7]
  Methyl ester bicyclo[1.1.0]butane-1-carboxylic acid
  Group-member nr.: 45-020

$C_6H_8O_4$
- Dimethyl (*Z*)-2-butenedioate [624-48-6]
  Dimethyl ester (*Z*)-2-butenedioic acid
  Dimethyl *cis*-2-butenedioate
  Dimethyl maleate
  Group-member nr.: 45-021
- 3,6-Dimethyl-1,4-dioxane-2,5-dione [95-96-5]
  Group-member nr.: 47-018

C_6H_8S
- 2,5-Dimethylthiophene [638-02-8]
  Group-member nr.: 53-011

C_6H_9N
- Cyclopentanecarbonitrile [4254-02-8]
  Cyclopentyl cyanide
  Cyanocyclopentane
  Group-member nr.: 32-019
- 2,4-Dimethyl-1*H*-pyrrole [625-82-1]
  Group-member nr.: 33-016
- 2,5-Dimethyl-1*H*-pyrrole [625-84-3]
  Group-member nr.: 33-017

C_6H_{10}
- Cyclohexene [110-83-8]
  1,2,3,4-Tetrahydrobenzene
  Group-member nr.: 14-006
- 1,5-Hexadiene [592-42-7]
  Diallyl
  Group-member nr.: 13-025
- 1-Methylcyclopentene [693-89-0]
  Group-member nr.: 14-007
- 3-Methylcyclopentene [1120-62-3]
  Group-member nr.: 14-008

$C_6H_{10}O$
- Cyclohexanone [108-94-1]
  Pimelic ketone
  Ketohexamethylene
  Group-member nr.: 43-017
- 4-Methyl-3-penten-2-one [141-79-7]
  Mesityl oxide
  Group-member nr.: 43-018
- 7-Oxabicyclo[4.1.0]heptane [286-20-4]
  1,2-Epoxycyclohexane
  Cyclohexene oxide
  Group-member nr.: 46-017

$C_6H_{10}O_2$
- Ethyl cyclopropanecarboxylate [4606-07-9]
  Ethyl ester cyclopropanecarboxylic acid
  Group-member nr.: 45-022
- Methyl cyclobutanecarboxylate [765-85-5]
  Methyl ester cyclobutanecarboxylic acid
  Group-member nr.: 45-023
- 2-Oxepanone [502-44-3]
  ϵ-Caprolactone
  6-Hexanolide
  Group-member nr.: 47-019
- 2-Propenyl propanoate [2408-20-0]
  Allyl propionate
  Group-member nr.: 45-024

$C_6H_{10}O_3$
- Ethyl ester 3-oxobutanoic acid [141-97-9]
  Ethyl 3-oxobutanoate
  Ethyl acetoacetate
  Ethyl ester acetoacetic acid
  Group-member nr.: 47-020

$C_6H_{10}O_4$
- Diethyl ethanedioate [95-92-1]
  Diethyl ester ethanedioic acid
  Diethyl oxalate
  Group-member nr.: 45-025
- 1,2-Ethanediyl diacetate [111-55-7]
  1,2-Ethanediyl ester acetic acid
  Ethylene glycol diacetate
  Group-member nr.: 45-026
- Hexanedioic acid [124-04-9]
  Adipic acid
  1,4-Butanedicarboxylic acid
  Group-member nr.: 44-013

$C_6H_{11}N$
- Hexanenitrile [628-73-9]
  Capronitrile
  Amyl cyanide
  Group-member nr.: 32-020

$C_6H_{11}NO$
- Cyclohexanone oxime [100-64-1]
  Group-member nr.: 62-052
- Hexahydro-2*H*-azepin-2-one [105-60-2]
  ϵ-Caprolactam
  6-Hexanelactam
  6-Aminohexanoic lactam
  Group-member nr.: 62-053

$C_6H_{11}NO_2$
- 4,4-Dimethoxybutanenitrile [14618-78-1]
  β-Cyanopropionaldehyde dimethyl acetal
  Group-member nr.: 62-054

C_6H_{12}
- Cyclohexane [110-82-7]
  Hexamethylene
  Group-member nr.: 12-007
- 2,3-Dimethyl-2-butene [563-79-1]
  Tetramethylethylene
  Group-member nr.: 13-026
- 3,3-Dimethyl-1-butene [558-37-2]
  tert-Butylethylene
  Neohexene
  Group-member nr.: 13-027
- 1-Hexene [592-41-6]
  Hexylene
  Group-member nr.: 13-028
- (Z)-2-Hexene [7688-21-3]
  cis-2-Hexene
  Group-member nr.: 13-029
- Methylcyclopentane [96-37-7]
  Group-member nr.: 12-008

$C_6H_{12}BNO_3$
- 2,8,9-Trioxa-5-aza-1-borabicyclo[3.3.3]-undecane [283-56-7]
  2,2',2''-Nitrilotriethanol cyclic ester with boric acid (1:1)
  Triethanolamine borate
  Group-member nr.: 72-007

$C_6H_{12}Cl_2$
- 1,6-Dichlorohexane [2163-00-0]
  Hexamethylene chloride
  Group-member nr.: 22-040

$C_6H_{12}Cl_3O_4P$
- 2-Chloroethanol phosphate (3:1) [115-96-8]
  Tri(2-chloroethyl)phosphate
  Group-member nr.: 72-008

$C_6H_{12}N_2$
- 1,4-Diazobicyclo[2.2.2]octane [280-57-9]
  Triethylenediamine
  Group-member nr.: 33-018
- (1-Methylethylidene)hydrazone 2-propanone [627-70-3]
  Acetone azine
  Dimethyl ketazine
  Group-member nr.: 34-008

$C_6H_{12}O$
- Cyclohexanol [108-93-0]
  Cyclohexyl alcohol
  Hexahydrophenol
  Group-member nr.: 42-038
- 3,3-Dimethyl-2-butanone [75-97-8]
  tert-Butyl methyl ketone
  Pinacolone
  Group-member nr.: 43-019
- 1-(Ethenyloxy)butane [111-34-2]
  Butyl vinyl ether
  Butoxyethylene
  Group-member nr.: 41-013
- 1-(Ethenyloxy)-2-methylpropane [109-53-5]
  Isobutyl vinyl ether
  Isobutoxyethylene
  Group-member nr.: 41-014
- Hexanal [66-25-1]
  Hexaldehyde
  Caproaldehyde
  Group-member nr.: 43-020
- 2-Hexanone [591-78-6]
  Butyl methyl ketone
  Group-member nr.: 43-021
- 3-Hexanone [589-38-8]
  Ethyl propyl ketone
  Group-member nr.: 43-022
- 4-Methyl-2-pentanone [108-10-1]
  Isobutyl methyl ketone
  Group-member nr.: 43-023

$C_6H_{12}O_2$
- Butyl acetate [123-86-4]
  Butyl ethanoate
  Group-member nr.: 45-027
- 1,1-Dimethylethyl acetate [540-88-5]
  1,1-Dimethylethyl ethanoate
  tert-Butyl acetate
  Group-member nr.: 45-028
- Ethyl butanoate [105-54-4]
  Ethyl butyrate
  Group-member nr.: 45-029
- Ethyl 2-methylpropanoate [97-62-1]
  Ethyl isobutyrate
  Group-member nr.: 45-030
- Hexanoic acid [142-62-1]
  Caproic acid
  Group-member nr.: 44-014
- 3-Methylbutyl formate [110-45-2]
  3-Methylbutyl methanoate
  Isoamyl formate
  Isopentyl formate
  Group-member nr.: 45-033
- Methyl 2,2-dimethylpropanoate [598-98-1]
  Methyl ester 2,2-dimethylpropanoic acid
  Methyl pivalate
  Methyl trimethylacetate
  Group-member nr.: 45-031
- Methyl pentanoate [624-24-8]
  Methyl valerate
  Group-member nr.: 45-032
- 2-Methylpropyl acetate [110-19-0]
  2-Methylpropyl ethanoate
  Isobutyl acetate
  Group-member nr.: 45-034
- Propyl propanoate [106-36-5]
  Propyl propionate
  Group-member nr.: 45-035
- Tetrahydro-2*H*-pyran-2-methanol [100-72-1]
  Group-member nr.: 47-021

$C_6H_{12}O_3$
- 2-Ethoxyethanol acetate [111-15-9]
  2-Ethoxyethyl acetate
  Cellosolve acetate
  Group-member nr.: 47-022
- 2,4,6-Trimethyl-1,3,5-trioxane [123-63-7]
  Paraldehyde
  Group-member nr.: 46-018

$C_6H_{12}S$
- Cyclohexanethiol [1569-69-3]
  Cyclohexyl mercaptan
  Group-member nr.: 52-015
- Methylthiocyclopentane [7133-36-0]
  Cyclopentyl methyl sulfide
  Group-member nr.: 51-013

$C_6H_{13}Br$
- 1-Bromohexane [111-25-1]
  n-Hexyl bromide
  Group-member nr.: 23-034
- 3-Bromohexane [3377-87-5]
  Group-member nr.: 23-035

$C_6H_{13}N$
- Cyclohexanamine [108-91-8]
  Cyclohexylamine
  Group-member nr.: 31-022
- Hexahydro-1*H*-azepine [111-49-9]
  Perhydroazepine
  Hexamethylenimine
  Azacycloheptane
  Group-member nr.: 33-019
- 1-Methylpiperidine [626-67-5]
  N-Methylpiperidine
  Group-member nr.: 33-020
- 2-Methylpiperidine [109-05-7]
  2-Pipecoline
  α-Pipecoline
  Group-member nr.: 33-021
- 4-Methylpiperidine [626-58-4]
  4-Pipecoline
  β-Pipecoline
  Group-member nr.: 33-022

$C_6H_{13}NO$
- *N*-Butylacetamide [1119-49-9]
  N-Butylethanamide
  Group-member nr.: 62-055
- *N*, *N*-Diethylacetamide [685-91-6]
  N, *N*-Diethylethanamide
  Group-member nr.: 62-056
- *N*-Methylpentanamide [6225-10-1]
  N-Methylvaleramide
  Group-member nr.: 62-057

C_6H_{14}
- 2,2-Dimethylbutane [75-83-2]
  Neohexane
  Group-member nr.: 11-011
- 2,3-Dimethylbutane [79-29-8]
  Diisopropyl
  Group-member nr.: 11-012
- Hexane [110-54-3]
  Group-member nr.: 11-013
- 2-Methylpentane [107-83-5]
  Dimethylpropylmethane
  Group-member nr.: 11-014
- 3-Methylpentane [96-14-0]
  Diethylmethylmethane
  Group-member nr.: 11-015

$C_6H_{14}N_2O$
- Dipropyldiazene 1-oxide [17697-55-1]
  Group-member nr.: 62-058

$C_6H_{14}O$
- 3,3-Dimethyl-1-butanol [624-95-3]
  Group-member nr.: 42-039
- 2-Ethoxy-2-methylpropane [637-92-3]
  tert-Butyl ethyl ether
  Group-member nr.: 41-015
- 2-Ethyl-1-butanol [97-95-0]
  2-Ethylbutyl alcohol
  Group-member nr.: 42-040
- 1-Hexanol [111-27-3]
  Hexyl alcohol
  Group-member nr.: 42-041
- 2-Hexanol [626-93-7]
  Group-member nr.: 42-042
- 3-Hexanol [623-37-0]
  Ethyl propyl carbinol
  Group-member nr.: 42-043
- 2-Methoxy-2-methylbutane [994-05-8]
  Methyl *tert*-pentyl ether
  3,3-Dimethyl-2-oxapentane
  tert-Amyl methyl ether
  Group-member nr.: 41-016
- 2-Methyl-1-pentanol [105-30-6]
  Group-member nr.: 42-044
- 2-Methyl-2-pentanol [590-36-3]
  Group-member nr.: 42-045
- 3-Methyl-2-pentanol [565-60-6]
  Group-member nr.: 42-046
- 3-Methyl-3-pentanol [77-74-7]
  Group-member nr.: 42-047
- 4-Methyl-2-pentanol [108-11-2]
  Group-member nr.: 42-048
- 1,1'-Oxybispropane [111-43-3]
  Dipropyl ether
  Group-member nr.: 41-017
- 2,2'-Oxybispropane [108-20-3]
  1,1'-Bis(methylethyl) ether
  Diisopropyl ether
  Group-member nr.: 41-018

$C_6H_{14}O_2$
- 2-Butoxyethanol [111-76-2]
  3-Oxa-1-heptanol
  Ethylene glycol monobutyl ether
  Butyl cellosolve
  Group-member nr.: 47-023
- 1,1-Diethoxyethane [105-57-7]
  Acetaldehyde diethyl acetal
  Acetal
  Group-member nr.: 41-019
- 1,2-Diethoxyethane [629-14-1]
  3,6-Dioxaoctane
  Ethylene glycol diethyl ether
  Diethyl cellosolve
  Group-member nr.: 41-020
- 1-Methoxy-2-propoxyethane [17081-22-0]
  2,5-Dioxaoctane
  Ethylene glycol methyl ether propyl ether
  Group-member nr.: 41-021

$C_6H_{14}O_3$
- 2-(2-Ethoxyethoxy)ethanol [111-90-0]
  Diethylene glycol monoethyl ether
  Group-member nr.: 47-024
- 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol [77-99-6]
  1,1,1-Tris(hydroxymethyl)propane
  Trimethylolpropane
  Group-member nr.: 42-049
- 1,1'-Oxybis(2-methoxyethane) [111-96-6]
  2,5,8-Trioxanonane
  Diethylene glycol dimethyl ether
  Diglyme
  Group-member nr.: 41-022

$C_6H_{14}O_4$
- 2,2'-[1,2-Ethanediylbis(oxy)]bisethanol [112-27-6]
  1,8-Dihydroxy-3,6-dioxaoctane
  Triethylene glycol
  Group-member nr.: 47-025

$C_6H_{14}O_6$
- *D*-Mannitol [69-65-8]
  Group-member nr.: 42-050

$C_6H_{14}S$
- 1-Hexanethiol [111-31-9]
  1-Hexyl mercaptan
  Group-member nr.: 52-016
- 2-(Methylthio)pentane [13286-91-4]
  3-Methyl-2-thiahexane
  Methyl 1-methylbutyl sulfide
  Group-member nr.: 51-014
- 1,1'-Thiobispropane [111-47-7]
  Dipropyl sulfide
  Group-member nr.: 51-015
- 2,2'-Thiobispropane [625-80-9]
  Bis(1-methylethyl) sulfide
  Diisopropyl sulfide
  Group-member nr.: 51-016

$C_6H_{14}S_2$
- Dipropyl disulfide [629-19-6]
  4,5-Dithiaoctane
  Group-member nr.: 51-017

$C_6H_{15}Al$
- Triethylaluminium [97-93-8]
  Group-member nr.: 73-018

$C_6H_{15}As$
- Triethylarsine [617-75-4]
  Group-member nr.: 73-019

$C_6H_{15}B$
- Triethylborane [97-94-9]
  Group-member nr.: 72-009

$C_6H_{15}Bi$
- Triethylbismuthine [617-77-6]
  Group-member nr.: 73-020

$C_6H_{15}ClSi$
- Chlorotriethylsilane [994-30-9]
  Group-member nr.: 71-012

$C_6H_{15}Ga$
- Triethylgallium [1115-99-7]
  Group-member nr.: 73-021

$C_6H_{15}In$
- Triethylindium [923-34-2]
  Group-member nr.: 73-022

$C_6H_{15}N$
- *N*, *N*-Diethylethanamine [121-44-8]
  Triethylamine
  Group-member nr.: 31-023
- 1-Hexanamine [111-26-2]
  Hexylamine
  Group-member nr.: 31-024
- *N*-Propyl-1-propanamine [142-84-7]
  Dipropylamine
  Group-member nr.: 31-025

$C_6H_{15}NO_3$
- 2,2',2''-Nitrilotrisethanol [102-71-6]
  Tri(2-hydroxyethyl)amine
  Triethanolamine
  Group-member nr.: 62-059

$C_6H_{15}N_3$
- 1-Piperazineethanamine [140-31-8]
  1-(2-Aminoethyl)piperazine
  Group-member nr.: 33-023

$C_6H_{15}Sb$
- Triethylstibine [617-85-6]
  Triethylantimony
  Group-member nr.: 73-023

$C_6H_{16}Si_2$
- 1,1,3,3-Tetramethyl-1,3-disilacyclobutane [1627-98-1]
  Group-member nr.: 71-013

$C_6H_{18}BN$
- Triethylamineborane [1722-26-5]
  N, *N*-Dimethylethanamine compd. with borane (1:1)
  Group-member nr.: 72-010

$C_6H_{18}N_3OP$
- Hexamethyl phosphoric triamide [680-31-9]
  Hexamethylphosphoramide
  Group-member nr.: 72-011

$C_6H_{18}N_4$
- *N*, *N*'-Bis(2-aminoethyl)-1,2-ethanediamine [112-24-3]
  Triethylenetetramine
  Group-member nr.: 31-026

$C_6H_{18}OSi_2$
- Hexamethyldisiloxane [107-46-0]
  Group-member nr.: 71-014

$C_6H_{18}O_3Si_3$
- Hexamethylcyclotrisiloxane [541-05-9]
  Group-member nr.: 71-015

$C_6H_{18}Si_2$
- Hexamethyldisilane [1450-14-2]
  Group-member nr.: 71-016

$C_6H_{21}N_3Si_3$
- 2,2,4,4,6,6-Hexamethylcyclotrisilazane [1009-93-4]
  Dimethylaminosilane trimer
  Group-member nr.: 71-017

C_7F_8
- Pentafluoro(trifluoromethyl)benzene [434-64-0]
  Octafluorotoluene
  Perfluorotoluene
  Group-member nr.: 21-020

C_7F_{14}
- (Trifluoromethyl)undecafluorocyclohexane [355-02-2]
  Perfluoromethylcyclohexane
  Group-member nr.: 21-021

C_7F_{16}
- Hexadecafluoroheptane [335-57-9]
  Perfluoroheptane
  Group-member nr.: 21-022

$C_7H_3F_5$
- Pentafluoromethylbenzene [771-56-2]
  2,3,4,5,6-Pentafluorotoluene
  Group-member nr.: 21-023

C_7H_4ClNO
- 1-Chloro-3-isocyanatobenzene [2909-38-8]
  m-Chlorophenylisocyanate
  Group-member nr.: 64-021

$C_7H_4F_3NO_2$
- 1-Nitro-3-(trifluoromethyl)benzene [98-46-4]
  m-Trifluoromethylnitrobenzene
  Group-member nr.: 64-022

C_7H_5ClO
- Benzoyl chloride [98-88-4]
  Group-member nr.: 61-039

$C_7H_5ClO_2$
- 2-Chlorobenzoic acid [118-91-2]
  o-Chlorobenzoic acid
  Group-member nr.: 61-040
- 3-Chlorobenzoic acid [535-80-8]
  m-Chlorobenzoic acid
  Group-member nr.: 61-041
- 4-Chlorobenzoic acid [74-11-3]
  p-Chlorobenzoic acid
  Group-member nr.: 61-042

$C_7H_5F_3$
- (Trifluoromethyl)benzene [98-08-8]
  α,α,α-Trifluorotoluene
  Group-member nr.: 21-024

C_7H_5N
- Benzonitrile [100-47-0]
  Phenyl cyanide
  Group-member nr.: 32-021

C_7H_5NO
- Benzoxazole [273-53-0]
  Group-member nr.: 62-060

$C_7H_5NO_4$
- 2-Nitrobenzoic acid [552-16-9]
  o-Nitrobenzoic acid
  o-Nitrodracylic acid
  Group-member nr.: 62-061
- 3-Nitrobenzoic acid [121-92-6]
  m-Nitrobenzoic acid
  m-Nitrodracylic acid
  Group-member nr.: 62-062
- 4-Nitrobenzoic acid [62-23-7]
  p-Nitrobenzoic acid
  p-Nitrodracylic acid
  Group-member nr.: 62-063

C_7H_5NS
- Benzothiazole [95-16-9]
  Group-member nr.: 64-023
- Isothiocyanatobenzene [103-72-0]
  Phenyl ester isothiocyanic acid
  Group-member nr.: 64-024

$C_7H_5N_3O_6$
- 2-Methyl-1,3,5-trinitrobenzene [118-96-7]
  2,4,6-Trinitrotoluene
  Tritol
  TNT
  Group-member nr.: 62-064

$C_7H_5N_5O_8$
- *N*-Methyl-*N*,2,4,6-tetranitrobenzenamine [479-45-8]
  Trinitrophenylmethylnitroamine
  Tetryl
  Group-member nr.: 62-065

$C_7H_6F_8O_3$
- Bis(2,2,3,3-tetrafluoropropyl) ester carbonic acid [1422-70-4]
  Bis(2,2,3,3-tetrafluoropropyl) carbonate
  Group-member nr.: 61-043

$C_7H_6N_2O_4$
- 2-Methyl-1,3-dinitrobenzene [606-20-2]
  2,6-Dinitrotoluene
  Group-member nr.: 62-066

C_7H_6O
- Benzaldehyde [100-52-7]
  Benzoic aldehyde
  Group-member nr.: 43-024

$C_7H_6O_2$
- Benzoic acid [65-85-0]
  Benzenecarboxylic acid
  Carboxybenzene
  Phenylformic acid
  Group-member nr.: 44-015
- 2-Hydroxybenzaldehyde [90-02-8]
  Salicyl aldehyde
  Group-member nr.: 47-026

$C_7H_6O_3$
- 2-Hydroxybenzoic acid [69-72-7]
  Salicylic acid
  Group-member nr.: 47-027

C_7H_7Cl
- (Chloromethyl)benzene [100-44-7]
  Benzyl chloride
  Group-member nr.: 22-041
- 1-Chloro-2-methylbenzene [95-49-8]
  2-Chlorotoluene
  o-Chlorotoluene
  o-Tolyl chloride
  Group-member nr.: 22-042

C_7H_7F
- 1-Fluoro-2-methylbenzene [95-52-3]
  2-Fluorotoluene
  o-Tolyl fluoride
  Group-member nr.: 21-025
- 1-Fluoro-3-methylbenzene [352-70-5]
  3-Fluorotoluene
  m-Tolyl fluoride
  Group-member nr.: 21-026
- 1-Fluoro-4-methylbenzene [352-32-9]
  p-Fluorotoluene
  p-Tolyl fluoride
  Group-member nr.: 21-027

C_7H_7NO
- Benzamide [55-21-0]
  Group-member nr.: 62-067

$C_7H_7NO_2$
- 1-Methyl-3-nitrobenzene [99-08-1]
  m-Nitrotoluene
  Group-member nr.: 62-068
- 1-Methyl-4-nitrobenzene [99-99-0]
  p-Nitrotoluene
  Group-member nr.: 62-069

$C_7H_7NO_3$
- 1-Methoxy-2-nitrobenzene [91-23-6]
  o-Nitroanisole
  Group-member nr.: 62-070
- 1-Methoxy-3-nitrobenzene [555-03-3]
  m-Nitroanisole
  Group-member nr.: 62-071
- 1-Methoxy-4-nitrobenzene [100-17-4]
  p-Nitroanisole
  Group-member nr.: 62-072

C_7H_8
- Bicyclo[2.2.1]hepta-2,5-diene [121-46-0]
  2,5-Norbornadiene
  Group-member nr.: 14-009
- 1,3,5-Cycloheptatriene [544-25-2]
  Group-member nr.: 14-010
- Methylbenzene [108-88-3]
  Toluene
  Phenyl methane
  Group-member nr.: 14-011
- Tetracyclo[3.2.0.$0^{2,7}$.$0^{4,6}$]heptane [278-06-8]
  Quadricyclane
  Group-member nr.: 12-009

$C_7H_8Cl_2Si$
- Dichloromethylphenylsilane [149-74-6]
  Group-member nr.: 71-018

C_7H_8O
- Benzenemethanol [100-51-6]
  Benzyl alcohol
  Group-member nr.: 42-051
- Methoxybenzene [100-66-3]
  Methyl phenyl ether
  Anisole
  Group-member nr.: 41-023
- 2-Methylphenol [95-48-7]
  o-Hydroxytoluene
  o-Cresol
  Group-member nr.: 42-052
- 3-Methylphenol [108-39-4]
  m-Hydroxytoluene
  m-Cresol
  Group-member nr.: 42-053
- 4-Methylphenol [106-44-5]
  p-Hydroxytoluene
  p-Cresol
  Group-member nr.: 42-054

$C_7H_8O_2$
- 2,6-Dimethyl-4*H*-pyran-4-one [1004-36-0]
  2,6-Dimethyl-β-pyrone
  Group-member nr.: 47-028

C_7H_8S
- Methylthiobenzene [100-68-5]
  Methyl phenyl sulfide
  Group-member nr.: 51-018

C_7H_9N
- Benzenemethanamine [100-46-9]
  Benzylamine
  Phenylmethylamine
  Aminotoluene
  Group-member nr.: 31-027
- Bicyclo[3.1.0]hexane-1-carbonitrile [31357-72-9]
  1-Bicyclo[3.1.0]hexyl cyanide
  1-Cyanobicyclo[3.1.0]hexane
  Group-member nr.: 32-022
- 2,3-Dimethylpyridine [583-61-9]
  2,3-Lutidine
  Group-member nr.: 33-024
- 2,4-Dimethylpyridine [108-47-4]
  2,4-Lutidine
  Group-member nr.: 33-025
- 2,5-Dimethylpyridine [589-93-5]
  2,5-Lutidine
  Group-member nr.: 33-026
- 2,6-Dimethylpyridine [108-48-5]
  2,6-Lutidine
  Group-member nr.: 33-027
- 3,4-Dimethylpyridine [583-58-4]
  3,4-Lutidine
  Group-member nr.: 33-028
- 3,5-Dimethylpyridine [591-22-0]
  3,5-Lutidine
  Group-member nr.: 33-029
- *N*-Methylbenzenamine [100-61-8]
  N-Methylaniline
  Methylphenylamine
  Group-member nr.: 31-028
- 2-Methylbenzenamine [95-53-4]
  2-Methylaniline
  o-Toluidine
  Group-member nr.: 31-029
- 3-Methylbenzenamine [108-44-1]
  3-Methylaniline
  m-Toluidine
  Group-member nr.: 31-030
- 4-Methylbenzenamine [106-49-0]
  4-Methylaniline
  p-Toluidine
  Group-member nr.: 31-031

$C_7H_{11}N$
- Cyclohexanecarbonitrile [766-05-2]
  Cyclohexyl cyanide
  Cyanocyclohexane
  Group-member nr.: 32-023

C_7H_{12}
- Bicyclo[4.1.0]heptane [286-08-8]
  Norcarane
  Group-member nr.: 12-010
- (*Z*)-Cycloheptene [45510-00-7]
  cis-Cycloheptene
  Group-member nr.: 14-012
- 1-Ethylcyclopentene [2146-38-5]
  Group-member nr.: 14-013
- Ethylidenecyclopentane [2146-37-4]
  Group-member nr.: 12-011
- 4-Methylcyclohexene [591-47-9]
  Group-member nr.: 14-014
- Methylenecyclohexane [1192-37-6]
  Group-member nr.: 12-012

$C_7H_{12}O$
- Cycloheptanone [502-42-1]
  Suberone
  Group-member nr.: 43-025
- 2-Methylcyclohexanone [583-60-8]
  o-Methylcyclohexanone
  Group-member nr.: 43-026
- 3-Methylcyclohexanone [591-24-2]
  m-Methylcyclohexanone
  Group-member nr.: 43-027
- 4-Methylcyclohexanone [589-92-4]
  p-Methylcyclohexanone
  Group-member nr.: 43-028

$C_7H_{12}O_2$
- Butyl 2-propenoate [141-32-2]
  Butyl ester 2-propenoic acid
  Butyl acrylate
  Group-member nr.: 45-036

- 2-Propenyl butanoate [2051-78-7]
  Allyl butyrate
  Group-member nr.: 45-037
- 2-Propenyl 2-methylpropanoate [15727-77-2]
  2-Propenyl ester 2-methylpropanoic acid
  Allyl isobutyrate
  Group-member nr.: 45-038

$C_7H_{12}O_4$
- Diethyl propanedioate [105-53-3]
  Diethyl ester propanedioic acid
  Diethyl malonate
  Group-member nr.: 45-039

$C_7H_{13}NO$
- Hexahydro-2(1*H*)-azocinone [673-66-5]
  β-Enantholactam
  Group-member nr.: 62-073

C_7H_{14}
- Cycloheptane [291-64-5]
  Group-member nr.: 12-013
- 1,1-Dimethylcyclopentane [1638-26-2]
  Group-member nr.: 12-014
- *cis*-1,2-Dimethylcyclopentane [1192-18-3]
  Group-member nr.: 12-015
- *trans*-1,2-Dimethylcyclopentane [822-50-4]
  Group-member nr.: 12-016
- *trans*-1,3-Dimethylcyclopentane [1759-58-6]
  Group-member nr.: 12-017
- Ethylcyclopentane [1640-89-7]
  Group-member nr.: 12-018
- 1-Heptene [592-76-7]
  1-Heptylene
  Group-member nr.: 13-030
- Methylcyclohexane [108-87-2]
  Hexahydrotoluene
  Group-member nr.: 12-019

$C_7H_{14}ClNO$
- Dipropylcarbamic chloride [27086-19-7]
  N, *N*-Dipropylcarbamoyl chloride
  Group-member nr.: 64-025

$C_7H_{14}O$
- Cycloheptanol [502-41-0]
  Group-member nr.: 42-055
- 3,4-Dimethylpentanal [19353-21-0]
  3,4-Dimethylvaleraldehyde
  Group-member nr.: 43-029
- 2,4-Dimethyl-3-pentanone [565-80-0]
  Diisopropyl ketone
  Group-member nr.: 43-030
- Heptanal [111-71-7]
  Heptyl aldehyde
  Enanthaldehyde
  Group-member nr.: 43-031
- 2-Heptanone [110-43-0]
  Methyl pentyl ketone
  Group-member nr.: 43-032
- 4-Heptanone [123-19-3]
  Dipropyl ketone
  Group-member nr.: 43-033
- 1-Methylcyclohexanol [590-67-0]
  Group-member nr.: 42-056
- 2-Methylcyclohexanol [583-59-5]
  o-Methylcyclohexanol (unspecified stereoisomer and chirality)
  Group-member nr.: 42-057
- *cis*-2-Methylcyclohexanol [7443-70-1]
  Group-member nr.: 42-058
- *trans*-2-Methylcyclohexanol [7443-52-9]
  Group-member nr.: 42-059
- 3-Methylcyclohexanol [591-23-1]
  m-Methylcyclohexanol (unspecified stereoisomer and chirality)
  Group-member nr.: 42-060
- 4-Methylcyclohexanol [589-91-3]
  p-Methylcyclohexanol (unspecified stereoisomer)
  Group-member nr.: 42-061
- 3-Methylhexanal [19269-28-4]
  Group-member nr.: 43-034
- 2-Methyl-3-hexanone [7379-12-6]
  Group-member nr.: 43-035

$C_7H_{14}O_2$
- Ethyl 2,2-dimethylpropanoate [3938-95-2]
  Ethyl ester 2,2-dimethylpropanoic acid
  Ethyl pivalate
  Group-member nr.: 45-040
- Ethyl 3-methylbutanoate [108-64-5]
  Ethyl isovalerate
  Group-member nr.: 45-041
- Ethyl pentanoate [539-82-2]
  Ethyl valerate
  Group-member nr.: 45-042
- Heptanoic acid [111-14-8]
  Enanthic acid
  Group-member nr.: 44-016
- 3-Methylbutyl acetate [123-92-2]
  3-Methylbutyl ethanoate
  Isoamyl acetate
  Isopentyl acetate
  Group-member nr.: 45-043
- 2-Methylpropyl propanoate [540-42-1]
  Isobutyl propionate
  Group-member nr.: 45-044
- Pentyl acetate [628-63-7]
  Pentyl ethanoate
  Amyl acetate
  Group-member nr.: 45-045
- Propyl butanoate [105-66-8]
  Propyl butyrate
  Group-member nr.: 45-046
- Propyl 2-methylpropanoate [644-49-5]
  Propyl isobutyrate
  Group-member nr.: 45-047

$C_7H_{15}Br$
- 1-Bromoheptane [629-04-9]
  n-Heptyl bromide
  Group-member nr.: 23-036

$C_7H_{15}Cl$
- 3-Chloroheptane [999-52-0]
  Group-member nr.: 22-043

$C_7H_{15}N$
- Octahydroazocine [1121-92-2]
  Perhydroazocine
  Heptamethylenimine
  Group-member nr.: 33-030

C_7H_{16}
- 2,2-Dimethylpentane [590-35-2]
  Group-member nr.: 11-016
- 2,3-Dimethylpentane [565-59-3]
  Group-member nr.: 11-017
- 2,4-Dimethylpentane [108-08-7]
  Group-member nr.: 11-018
- 3,3-Dimethylpentane [562-49-2]
  Group-member nr.: 11-019
- 3-Ethylpentane [617-78-7]
  Triethylmethane
  Group-member nr.: 11-020
- Heptane [142-82-5]
  Dipropylmethane
  Group-member nr.: 11-021
- 2-Methylhexane [591-76-4]
  Isoheptane
  Ethylisobutylmethane
  Group-member nr.: 11-022
- 3-Methylhexane [589-34-4]
  Group-member nr.: 11-023
- 2,2,3-Trimethylbutane [464-06-2]
  Isopropyltrimethylmethane
  Triptane
  Group-member nr.: 11-024

$C_7H_{16}O$
- 2-Ethoxy-2-methylbutane [919-94-8]
  Ethyl *tert*-pentyl ether
  4,4-Dimethyl-3-oxahexane
  tert-Amyl ethyl ether
  Group-member nr.: 41-024
- 3-Ethyl-3-pentanol [597-49-9]
  Group-member nr.: 42-062
- 1-Heptanol [111-70-6]
  Heptyl alcohol
  Group-member nr.: 42-063
- 2-Heptanol [543-49-7]
  Group-member nr.: 42-064
- 4-Heptanol [589-55-9]
  Dipropyl carbinol
  Group-member nr.: 42-065

$C_7H_{16}O_2$
- 1-Butoxy-2-methoxyethane [13343-98-1]
  2,5-Dioxanonane
  Ethylene glycol butyl ether methyl ether
  Group-member nr.: 41-025
- 1,3-Diethoxypropane [3459-83-4]
  3,7-Dioxanonane
  Propylene glycol diethyl ether
  Group-member nr.: 41-026
- 1,5-Dimethoxypentane [111-89-7]
  2,8-Dioxanonane
  Pentylene glycol dimethyl ether
  Group-member nr.: 41-027
- 1-Ethoxy-4-methoxybutane [36865-47-1]
  2,7-Dioxanonane
  Butylene glycol ethyl ether methyl ether
  Group-member nr.: 41-028
- 1-Ethoxy-2-propoxyethane [18854-31-4]
  3,6-Dioxanonane
  Ethylene glycol ethyl ether propyl ether
  Group-member nr.: 41-029
- 1-Methoxy-3-propoxypropane [89851-49-0]
  2,6-Dioxanonane
  Propylene glycol methyl ether propyl ether
  Group-member nr.: 41-030

$C_7H_{16}O_3$
- 1,1',1''-[Methylidynetris(oxy)]trisethane [122-51-0]
  Triethoxymethane
  Triethyl ester orthoformic acid
  Triethyl orthoformate
  Group-member nr.: 41-031

$C_7H_{16}S$
- 1-Heptanethiol [1639-09-4]
  1-Heptyl mercaptan
  Group-member nr.: 52-017
- 2-(Methylthio)hexane [76858-84-9]
  3-Methyl-2-thiaheptane
  Methyl 1-methylpentyl sulfide
  Group-member nr.: 51-019

$C_7H_{20}Si_2$
- Methylenebis[trimethylsilane] [2117-28-4]
  2,2,4,4-Tetramethyl-2,4-disilapentane
  Hexamethyldisilamethane
  Bis(trimethylsilyl)methane
  Group-member nr.: 71-019

C_8F_{16}
- Decafluorobis(trifluoromethyl)cyclohexane [26637-68-3]
  Perfluorodimethylcyclohexane
  Hexadecafluorodimethyl-cyclohexane
  (unspecified isomer)
  Group-member nr.: 21-028

$C_8F_{16}O$
- 2,2,3,3,4,4,5,5-Heptafluorotetrahydro-4-(nonafluorobutyl)furan [646-85-5]
  Perfluoro-3-butyltetrahydrofuran
  Group-member nr.: 61-044

C_8F_{18}
- Octadecafluorooctane [307-34-6]
  Perfluorooctane
  Group-member nr.: 21-029

$C_8H_4Cl_2O_2$
- 1,2-Benzenedicarbonyl dichloride [88-95-9]
  Phthaloyl chloride
  Phthaloyl dichloride
  Group-member nr.: 61-045

$C_8H_4N_2$
- 1,2-Benzenedicarbonitrile [91-15-6]
  1,2-Dicyanobenzene
  Phthalonitrile
  Group-member nr.: 32-024

C_8H_6
- Ethynylbenzene [536-74-3]
  Phenylacetylene
  Group-member nr.: 14-015

C_8H_6O
- Benzofuran [271-89-6]
  Benzo[*b*]furan
  Cumaron
  Group-member nr.: 46-019

C_8H_6S
- Benzo[*b*]thiophene [95-15-8]
  Group-member nr.: 53-012

$C_8H_7N_5O_8$
- *N*-Ethyl-*N*,2,4,6-tetranitrobenzenamine [6052-13-7]
  Trinitrophenylethylnitroamine
  Ethyltetryl
  Group-member nr.: 62-074
- 3-Methyl-2,4,6-trinitro-*N*-(nitromethyl)benzenamine [43072-20-4]
  2,4,6-Trinitro-*N*-(methylnitro)-*m*-toluidine
  Methyltetryl
  Group-member nr.: 62-075

C_8H_8
- 1,3,5,7-Cyclooctatetraene [629-20-9]
  Group-member nr.: 14-016
- Ethenylbenzene [100-42-5]
  Vinylbenzene
  Styrene
  Group-member nr.: 14-017

C_8H_8O
- 2,3-Dihydrobenzofuran [496-16-2]
  Coumaran
  Group-member nr.: 46-020
- 1-Phenylethanone [98-86-2]
  Methyl phenyl ketone
  Acetophenone
  Acetyl benzene
  Hypnone
  Group-member nr.: 43-036

$C_8H_8O_2$
- Methyl benzoate [93-58-3]
  Methyl ester benzoic acid
  Group-member nr.: 45-048
- 2-Methylbenzoic acid [118-90-1]
  o-Toluic acid
  o-Toluylic acid
  Group-member nr.: 44-017
- 3-Methylbenzoic acid [99-04-7]
  m-Toluic acid
  Group-member nr.: 44-018
- 4-Methylbenzoic acid [99-94-5]
  p-Toluic acid
  Group-member nr.: 44-019

$C_8H_8O_3$
- Methyl 2-hydroxybenzoate [119-36-8]
  Methyl salicylate
  Group-member nr.: 47-029
- 3a,4,7,7a-Tetrahydro-1,3-isobenzofurandione [85-43-8]
  4-Cyclohexene-1,2-dicarboxylic acid anhydride
  1,2,3,6-Tetrahydrophthalic anhydride
  Group-member nr.: 44-020

$C_8H_9NO_2$
- *N*-(2-Hydroxyphenyl)acetamide [614-80-2]
  o-Hydroxyacetanilide
  Group-member nr.: 62-076
- Methyl ester phenylcarbamic acid [2603-10-3]
  Methyl phenylcarbamate
  Methyl ester carbanilic acid
  Group-member nr.: 62-077

C_8H_{10}
- 1,2-Dimethylbenzene [95-47-6]
  o-Xylene
  Group-member nr.: 14-018
- 1,3-Dimethylbenzene [108-38-3]
  m-Xylene
  Group-member nr.: 14-019
- 1,4-Dimethylbenzene [106-42-3]
  p-Xylene
  Group-member nr.: 14-020
- Ethylbenzene [100-41-4]
  Phenylethane
  Group-member nr.: 14-021

$C_8H_{10}N_2$
- Phenylhydrazone acetaldehyde [935-07-9]
  Group-member nr.: 34-009

$C_8H_{10}O$
- Benzeneethanol [60-12-8]
  Phenethyl alcohol
  2-Phenylethanol
  Group-member nr.: 42-066
- Ethoxybenzene [103-73-1]
  Ethyl phenyl ether
  Phenetole
  Group-member nr.: 41-032
- 1-Methoxy-4-methylbenzene [104-93-8]
  Methyl 4-methylphenyl ether
  p-Methylanisole
  Methyl *p*-tolyl ether
  p-Cresol methyl ether
  Group-member nr.: 41-033

$C_8H_{10}O_2$
- 2-Phenoxyethanol [122-99-6]
  Ethylene glycol monophenyl ether
  Group-member nr.: 47-030

$C_8H_{10}O_4$
- Di-2-propenyl ethanedioate [615-99-6]
  Di-2-propenyl ester ethanedioic acid
  Diallyl oxalate
  Group-member nr.: 45-049

$C_8H_{11}N$
- Benzeneethanamine [64-04-0]
  2-Phenylethylamine
  Phenethylamine
  Group-member nr.: 31-032
- *endo*-Bicyclo[2.2.1]heptane-2-carbonitrile [3211-87-8]
  endo-2-Cyanobicyclo[2.2.1]heptane
  endo-2-Norbornanecarbonitrile
  Group-member nr.: 32-025
- *exo*-Bicyclo[2.2.1]heptane-2-carbonitrile [3211-90-3]
  exo-2-Cyanobicyclo[2.2.1]heptane
  exo-2-Norbornanecarbonitrile
  Group-member nr.: 32-026
- *N*, *N*-Dimethylbenzenamine [121-69-7]
  N, *N*-Dimethylaniline
  Group-member nr.: 31-033
- 2,6-Dimethylbenzenamine [87-62-7]
  2,6-Dimethylaniline
  2,6-Xylidine
  Group-member nr.: 31-034
- 2,3,6-Trimethylpyridine [1462-84-6]
  2,3,6-Collidine
  Group-member nr.: 33-031
- 2,4,6-Trimethylpyridine [108-75-8]
  2,4,6-Collidine
  Group-member nr.: 33-032

C_8H_{12}
- Bicyclo[2.2.2]oct-2-ene [931-64-6]
  Group-member nr.: 14-022
- 1,5-Cyclooctadiene (unspecified stereoisomer) [111-78-4]
  Group-member nr.: 14-023

$C_8H_{12}N_2$
- 1,6-Diisocyanohexane [929-57-7]
  1,6-Hexamethylene isocyanide
  1,6-Hexamethylene diisocyanide
  Group-member nr.: 34-010

$C_8H_{12}N_2O_2$
- 1,6-Diisocyanatohexane [822-06-0]
  Hexamethylene diisocyanate
  Hexamethylene ester isocyanic acid
  Group-member nr.: 62-078

C_8H_{14}
- Bicyclo[2.2.2]octane [280-33-1]
  Group-member nr.: 12-020
- *cis*-Bicyclo[4.2.0]octane [28282-35-1]
  Group-member nr.: 12-021
- Cyclooctene (unspecified stereoisomer) [931-88-4]
  Group-member nr.: 14-024
- Ethylidenecyclohexane [1003-64-1]
  Group-member nr.: 12-022
- *endo*-2-Methylbicyclo[2.2.1]heptane [765-90-2]
  endo-2-Methylnorbornane
  Group-member nr.: 12-023
- *exo*-2-Methylbicyclo[2.2.1]heptane [872-78-6]
  exo-2-Methylnorbornane
  Group-member nr.: 12-024
- *cis*-Octahydropentalene [1755-05-1]
  cis-Bicyclo[3.3.0]octane
  Group-member nr.: 12-025
- *trans*-Octahydropentalene [5597-89-7]
  trans-Bicyclo[3.3.0]octane
  Group-member nr.: 12-026
- (2-Propenyl)cyclopentane [3524-75-2]
  Allylcyclopentane
  Group-member nr.: 12-027

$C_8H_{14}O$
- 6-Methyl-5-hepten-2-one [110-93-0]
  Group-member nr.: 43-037
- 3-Oxabicyclo[3.2.2]nonane [283-27-2]
  Group-member nr.: 46-021

$C_8H_{14}O_2$
- Butyl 2-methyl-2-propenoate [97-88-1]
  Butyl methacrylate
  Group-member nr.: 45-050
- 2-Propenyl pentanoate [6321-45-5]
  Allyl valerate
  Group-member nr.: 45-051

$C_8H_{14}O_4$
- Diethyl butanedioate [123-25-1]
  Diethyl ester butanedioic acid
  Diethyl succinate
  Group-member nr.: 45-052
- Dipropyl ethanedioate [615-98-5]
  Dipropyl ester ethanedioic acid
  Dipropyl oxalate
  Group-member nr.: 45-053
- 1,2-Ethanediyl dipropanoate [123-80-8]
  1,2-Ethanediyl ester propanoic acid
  Ethylene
  glycol dipropionate
  Group-member nr.: 45-054

$C_8H_{14}O_6$
- Diethyl ester 2,3-dihydroxy-[*R*-(*R**, *R**)]-butanedioic acid [87-91-2]
  Diethyl *L*(+)-tartarate
  Group-member nr.: 47-031

$C_8H_{15}N$
- 3-Azabicyclo[3.2.2]nonane [283-24-9]
  Group-member nr.: 33-033

C_8H_{16}
- Cyclooctane [292-64-8]
  Group-member nr.: 12-028
- 1,1-Dimethylcyclohexane [590-66-9]
  Group-member nr.: 12-029
- *cis*-1,2-Dimethylcyclohexane [2207-01-4]
  Group-member nr.: 12-030
- *trans*-1,2-Dimethylcyclohexane [6876-23-9]
  Group-member nr.: 12-031
- *cis*-1,3-Dimethylcyclohexane [638-04-0]
  Group-member nr.: 12-032
- *trans*-1,3-Dimethylcyclohexane [2207-03-6]
  Group-member nr.: 12-033
- *cis*-1,4-Dimethylcyclohexane [624-29-3]
  Group-member nr.: 12-034
- *trans*-1,4-Dimethylcyclohexane [2207-04-7]
  Group-member nr.: 12-035
- Ethylcyclohexane [1678-91-7]
  Group-member nr.: 12-036
- 1-Octene [111-66-0]
  1-Octylene
  1-Caprylene
  Group-member nr.: 13-031
- Propylcyclopentane [2040-96-2]
  Group-member nr.: 12-037
- 2,4,4-Trimethyl-1-pentene [107-39-1]
  Group-member nr.: 13-032
- 2,4,4-Trimethyl-2-pentene [107-40-4]
  Group-member nr.: 13-033

$C_8H_{16}O$
- Octanal [124-13-0]
  Octyl aldehyde
  Caprilic aldehyde
  Group-member nr.: 43-038
- 2-Octanone [111-13-7]
  Hexyl methyl ketone
  Group-member nr.: 43-039

$C_8H_{16}O_2$
- Butyl butanoate [109-21-7]
  Butyl butyrate
  Group-member nr.: 45-055
- Ethyl hexanoate [123-66-0]
  Ethyl caproate
  Group-member nr.: 45-056
- Hexyl acetate [142-92-7]
  Hexyl ethanoate
  Group-member nr.: 45-057
- 3-Methylbutyl propanoate [105-68-0]
  Isoamyl propionate
  Isopentyl propionate
  Group-member nr.: 45-059
- Methyl heptanoate [106-73-0]
  Methyl enanthoate
  Group-member nr.: 45-058
- 2-Methylpropyl butanoate [539-90-2]
  Isobutyl butyrate
  Group-member nr.: 45-060
- 2-Methylpropyl 2-methylpropanoate [97-85-8]
  Isobutyl isobutyrate
  Group-member nr.: 45-061
- Octanoic acid [124-07-2]
  Caprylic acid
  Group-member nr.: 44-021
- Pentyl propanoate [624-54-4]
  Amyl propionate
  Group-member nr.: 45-062
- Propyl pentanoate [141-06-0]
  Propyl valerate
  Group-member nr.: 45-063

$C_8H_{16}O_4$
- 2-(2-Ethoxyethoxy)ethanol acetate [112-15-2]
  2-(2-Ethoxyethoxy)ethyl acetate
  Diethylene glycol ethyl ether acetate
  Group-member nr.: 47-032
- 1,4,7,10-Tetraoxacyclododecane [294-93-9]
  Group-member nr.: 46-022

$C_8H_{17}Br$
- 1-Bromooctane [111-83-1]
  n-Octyl bromide
  Group-member nr.: 23-037

$C_8H_{17}NO$
- *N*, *N*-Dipropylacetamide [1116-24-1]
  Group-member nr.: 62-079

C_8H_{18}
- 2,3-Dimethylhexane [584-94-1]
  Group-member nr.: 11-025
- 2,5-Dimethylhexane [592-13-2]
  Group-member nr.: 11-026

- 3,3-Dimethylhexane [563-16-6]
  Group-member nr.: 11-027
- 3-Ethyl-2-methylpentane [609-26-7]
  Group-member nr.: 11-028
- 2-Methylheptane [592-27-8]
  Group-member nr.: 11-029
- 3-Methylheptane [589-81-1]
  Group-member nr.: 11-030
- 4-Methylheptane [589-53-7]
  Methyldipropylmethane
  Group-member nr.: 11-031
- Octane [111-65-9]
  Group-member nr.: 11-032
- 2,2,3,3-Tetramethylbutane [594-82-1]
  Group-member nr.: 11-033
- 2,2,4-Trimethylpentane [540-84-1]
  Isooctane
  Group-member nr.: 11-034
- 2,3,3-Trimethylpentane [560-21-4]
  Group-member nr.: 11-035
- 2,3,4-Trimethylpentane [565-75-3]
  Group-member nr.: 11-036

$C_8H_{18}N_2O$
- Bis(1,1-dimethylethyl)diazene 1-oxide [16649-52-8]
  Di-*tert*-butyldiazene *N*-oxide
  Group-member nr.: 62-080

$C_8H_{18}O$
- 2-Ethyl-1-hexanol [104-76-7]
  Group-member nr.: 42-067
- 2-Methyl-1-heptanol [106-67-2]
  Group-member nr.: 42-068
- 2-Methyl-2-heptanol [625-25-2]
  Group-member nr.: 42-069
- 2-Methyl-4-heptanol [21570-35-4]
  Group-member nr.: 42-070
- 3-Methyl-2-heptanol [31367-46-1]
  Group-member nr.: 42-071
- 4-Methyl-2-heptanol [56298-90-9]
  Group-member nr.: 42-072
- 4-Methyl-3-heptanol [14979-39-6]
  Group-member nr.: 42-073
- 4-Methyl-4-heptanol [598-01-6]
  Group-member nr.: 42-074
- 5-Methyl-1-heptanol [7212-53-5]
  Group-member nr.: 42-075
- 5-Methyl-2-heptanol [54630-50-1]
  Group-member nr.: 42-076
- 6-Methyl-2-heptanol [4730-22-7]
  Group-member nr.: 42-077
- 6-Methyl-3-heptanol [18720-66-6]
  Group-member nr.: 42-078
- 1-Octanol [111-87-5]
  Octyl alcohol
  Group-member nr.: 42-079
- 2-Octanol [123-96-6]
  Group-member nr.: 42-080
- 3-Octanol [589-98-0]
  Group-member nr.: 42-081
- 4-Octanol [589-62-8]
  Group-member nr.: 42-082
- 1,1'-Oxybisbutane [142-96-1]
  Dibutyl ether
  Group-member nr.: 41-034

$C_8H_{18}O_2$
- 1,2-Dipropoxyethane [18854-56-3]
  4,7-Dioxadecane
  Ethylene glycol dipropyl ether
  Group-member nr.: 41-035

$C_8H_{18}O_3$
- 2-(2-Butoxyethoxy)ethanol [112-34-5]
  Diethylene glycol monobutyl ether
  Group-member nr.: 47-033
- 1,1'-Oxybis(2-ethoxyethane) [112-36-7]
  3,6,9-Trioxaundecane
  Diethylene glycol diethyl ether
  Group-member nr.: 41-036

$C_8H_{18}O_4$
- 2,5,8,11-Tetraoxadodecane [112-49-2]
  Triethylene glycol dimethyl ether
  Triglyme
  Group-member nr.: 41-037

$C_8H_{18}O_5$
- 2,2'-[Oxybis(2,1-ethanediyloxy)]bisethanol [112-60-7]
  Tetraethylene glycol
  Group-member nr.: 47-034

$C_8H_{18}S$
- 2-(Methylthio)heptane [54063-12-6]
  3-Methyl-2-thiaoctane
  Methyl 1-methylhexyl sulfide
  Group-member nr.: 51-020
- 1,1'-Thiobisbutane [544-40-1]
  Dibutyl sulfide
  Group-member nr.: 51-021

$C_8H_{19}N$
- 2-Methyl-*N*-(2-methylpropyl)-1-propanamine [110-96-3]
  Diisobutylamine
  Group-member nr.: 31-035

$C_8H_{19}NSi$
- 1-[2-(Trimethylsilyl)ethyl]azetidine [42525-64-4]
  N-(β-Trimethylsilylethyl)trimethylenimine
  Group-member nr.: 71-020

$C_8H_{20}Ge$
- Tetraethylgermane [597-63-7]
  Group-member nr.: 73-024

$C_8H_{20}N_4$
- 1,4-Piperazinediethanamine [6531-38-0]
  1,4-Bis(2-aminoethyl)piperazine
  Group-member nr.: 33-034
- *N*-[2-(1-Piperazinyl)ethyl]-1,2-ethanediamine [24028-46-4]
  1-[2-[(2-Aminoethyl)amino]ethyl]piperazine
  Group-member nr.: 33-035

$C_8H_{20}O_4Si$
- Tetraethyl ester silicic acid [78-10-4]
  Tetraethyl orthosilicate
  Tetraethoxysilane
  Group-member nr.: 71-021

$C_8H_{20}Pb$
- Tetraethylplumbane [78-00-2]
  Tetraethyllead
  TEL
  Group-member nr.: 73-025

$C_8H_{20}Si$
- Tetraethylsilane [631-36-7]
  Group-member nr.: 71-022

$C_8H_{20}Sn$
- Tetraethylstannane [597-64-8]
  Tetraethyltin
  Group-member nr.: 73-026

$C_8H_{23}N_5$
- *N*-(2-Aminoethyl)-*N*'-[2-[(2-aminoethyl)amino]ethyl]-1,2-ethanediamine [112-57-2]
  Tetraethylenepentamine
  Group-member nr.: 31-036

$C_8H_{24}O_4Si_4$
- Octamethylcyclotetrasiloxane [556-67-2]
  Group-member nr.: 71-023

$C_8H_{28}N_4Si_4$
- 2,2,4,4,6,6,8,8-Octamethylcyclotetrasilazane [1020-84-4]
  Dimethylaminosilane tetramer
  Group-member nr.: 71-024

$C_9H_4O_5$
- 1,3-Dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid [552-30-7]
  1,2,4-Benzenetricarboxylic 1:2 anhydride
  Trimellitic anhydride
  Group-member nr.: 47-035

$C_9H_6N_2O_2$
- 2,4-Diisocyanato-1-methylbenzene [584-84-9]
  4-Methyl-*m*-phenyl diisocyanate
  4-Methyl-1,3-phenylene ester isocyanic acid
  2,4-Diisocyanate tolylene
  Group-member nr.: 62-081

C_9H_7ClO
- 2-Chloro-3-phenyl-2-propenal [18365-42-9]
  α-Chlorocinnamaldehyde
  Group-member nr.: 61-046

C_9H_7N
- Isoquinoline [119-65-3]
  Benzo[c]pyridine
  Group-member nr.: 33-036
- Quinoline [91-22-5]
  Benzo[*b*]pyridine
  Group-member nr.: 33-037

C_9H_8
- 1*H*-Indene [95-13-6]
  Group-member nr.: 14-025

C_9H_8O
- 3-Phenyl-2-propenal [104-55-2]
  Cinnamaldehyde
  Group-member nr.: 43-040

C_9H_{10}
- 2,3-Dihydroindene [496-11-7]
  Indan
  Group-member nr.: 14-026
- (1-Methylethenyl)benzene [98-83-9]
  Isopropenylbenzene
  α-Methylstyrene
  Group-member nr.: 14-027

$C_9H_{10}O$
- 3,4-Dihydro-1*H*-2-benzopyran [493-05-0]
  Isochroman
  Group-member nr.: 46-023
- 3,4-Dihydro-2*H*-1-benzopyran [493-08-3]
  Chroman
  Group-member nr.: 46-024
- 1-Phenyl-1-propanone [93-55-0]
  Ethyl phenyl ketone
  Propiophenone
  Group-member nr.: 43-041

$C_9H_{10}O_2$
- Ethyl benzoate [93-89-0]
  Ethyl ester benzoic acid
  Group-member nr.: 45-064
- (Phenoxymethyl)oxirane [122-60-1]
  Phenyl glycidyl ether
  Group-member nr.: 47-036
- Phenylmethyl acetate [140-11-4]
  Phenylmethyl ester acetic acid
  Benzyl acetate
  Group-member nr.: 45-065

$C_9H_{10}O_3$
- 3a,4,7,7a-Tetrahydro-4-methyl-1,3-isobenzofurandione [5333-84-6]
  3-Methyl-4-cyclohexene-1,2-dicarboxylic acid anhydride
  3-Methyl-1,2,3,6-tetrahydrophthalic anhydride
  Group-member nr.: 44-022

$C_9H_{11}N$
- 1,2,3,4-Tetrahydroquinoline [635-46-1]
  Group-member nr.: 33-038
- 5,6,7,8-Tetrahydroquinoline [10500-57-9]
  2,3-Cyclohexenopyridine
  Group-member nr.: 33-039

$C_9H_{11}NO_2$
- Ethyl ester phenylcarbamic acid [101-99-5]
  Ethyl phenylcarbamate
  Ethyl ester carbanilic acid
  Group-member nr.: 62-082

C_9H_{12}
- (1-Methylethyl)benzene [98-82-8]
  Isopropylbenzene
  Cumene
  Group-member nr.: 14-028
- Propylbenzene [103-65-1]
  Group-member nr.: 14-029
- 1,2,3-Trimethylbenzene [526-73-8]
  Hemimellitene
  Group-member nr.: 14-030
- 1,2,4-Trimethylbenzene [95-63-6]
  Pseudocumene
  Group-member nr.: 14-031
- 1,3,5-Trimethylbenzene [108-67-8]
  Mesitylene
  Group-member nr.: 14-032

$C_9H_{12}O$
- Benzenepropanol [122-97-4]
  3-Phenyl-1-propanol
  Phenylethyl carbinol
  Hydrocinnamyl alcohol
  Group-member nr.: 42-083
- 1-Ethoxy-4-methylbenzene [622-60-6]
  Ethyl-4-methylphenyl ether
  p-Methylphenetole
  Ethyl *p*-tolyl ether
  Group-member nr.: 41-038
- 1-Methoxy-2,4-dimethylbenzene [6738-23-4]
  Methyl 2,4-dimethylphenyl ether
  2,4-Dimethylanisole
  Group-member nr.: 41-039
- Propoxybenzene [622-85-5]
  Phenyl propyl ether
  Group-member nr.: 41-040

$C_9H_{13}N$
- Benzenepropanamine [2038-57-5]
  3-Phenylpropylamine
  Group-member nr.: 31-037
- *N*, *N*, 2-Trimethylbenzenamine [609-72-3]
  N, *N*-Dimethyl-*o*-toluidine
  Group-member nr.: 31-038

$C_9H_{14}O$
- 2,5,6-Trimethyl-2-cyclohexen-1-one [20030-30-2]
  Group-member nr.: 43-042

$C_9H_{14}O_6$
- 1,2,3-Propanetriol triacetate [102-76-1]
  1,2,3-Propanetriyl ester acetic acid
  Triacetin
  Group-member nr.: 45-066

C_9H_{16}
- *cis*-Bicyclo[6.1.0]nonane [13757-43-2]
  Group-member nr.: 12-038
- Octahydro-1*H*-indene [496-10-6]
  Hexahydroindan
  Hydrindan (unspecified stereoisomer)
  Group-member nr.: 12-039
- *cis*-Octahydro-1*H*-indene [4551-51-3]
  cis-Hexahydroindan
  cis-Hydrindan
  Group-member nr.: 12-040
- *trans*-Octahydro-1*H*-indene [3296-50-2]
  trans-Hexahydroindan
  trans-Hydrindan
  Group-member nr.: 12-041
- (2-Propenyl)cyclohexane [2114-42-3]
  Allylcyclohexane
  Group-member nr.: 12-042

$C_9H_{16}O_2$
- Ethyl cyclohexanecarboxylate [3289-28-9]
  Ethyl ester cyclohexanecarboxylic acid
  Group-member nr.: 45-067

$C_9H_{16}O_4$
- Dipropyl propanedioate [1117-19-7]
  Dipropyl ester propanedioic acid
  Dipropyl malonate
  Group-member nr.: 45-068

C_9H_{18}
- Butylcyclopentane [2040-95-1]
  Group-member nr.: 12-043
- 1-Nonene [124-11-8]
  Group-member nr.: 13-034
- Propylcyclohexane [1678-92-8]
  Group-member nr.: 12-044

$C_9H_{18}O$
- 2,6-Dimethyl-4-heptanone [108-83-8]
  Diisobutyl ketone
  Group-member nr.: 43-043
- Nonanal [124-19-6]
  Nonyl aldehyde
  Pelargonic aldehyde
  Group-member nr.: 43-044
- 5-Nonanone [502-56-7]
  Dibutyl ketone
  Group-member nr.: 43-045

$C_9H_{18}O_2$
- Butyl pentanoate [591-68-4]
  Butyl valerate
  Group-member nr.: 45-069
- 3-Methylbutyl butanoate [106-27-4]
  Isoamyl butyrate
  Isopentyl butyrate
  Group-member nr.: 45-071

- 3-Methylbutyl 2-methylpropanoate [2050-01-3]
  Isoamyl isobutyrate
  Isopentyl isobutyrate
  Group-member nr.: 45-072
- Methyl octanoate [111-11-5]
  Methyl caprylate
  Group-member nr.: 45-070
- 2-Methylpropyl pentanoate [10588-10-0]
  Isobutyl valerate
  Group-member nr.: 45-073
- Nonanoic acid [112-05-0]
  Pelargonic acid
  Group-member nr.: 44-023
- Pentyl butanoate [540-18-1]
  Pentyl butyrate
  Amyl butyrate
  Group-member nr.: 45-074

$C_9H_{19}Br$
- 1-Bromononane [693-58-3]
  n-Nonyl bromide
  Group-member nr.: 23-038

$C_9H_{19}NOS$
- *S*-Ethyl ester dipropylcarbamothionic acid [759-94-4]
  S-Ethyl dipropylthiocarbamate
  Group-member nr.: 64-026

C_9H_{20}
- 3,3-Diethylpentane [1067-20-5]
  Group-member nr.: 11-037
- Nonane [111-84-2]
  Group-member nr.: 11-038
- 2,2,3,3-Tetramethylpentane [7154-79-2]
  Group-member nr.: 11-039
- 2,2,4,4-Tetramethylpentane [1070-87-7]
  Group-member nr.: 11-040

$C_9H_{20}N_2O$
- Tetraethyl urea [1187-03-7]
  Tetraethylcarbamide
  Group-member nr.: 62-083

$C_9H_{20}O$
- 1-Nonanol [143-08-8]
  Nonyl alcohol
  Group-member nr.: 42-084

$C_9H_{21}Al$
- Tripropylaluminium [102-67-0]
  Group-member nr.: 73-027

$C_9H_{21}ClO_3Si$
- (3-Chloropropyl)triethoxysilane [5089-70-3]
  Group-member nr.: 71-025

$C_9H_{23}NO_3Si$
- 3-(Triethoxysilyl)-1-propanamine [919-30-2]
  3-(Triethoxysilyl)propylamine
  3-Aminopropyltriethoxysilane
  Group-member nr.: 71-026

$C_9H_{24}Si_2$
- 1,3-Propanediylbis[trimethylsilane] [2295-05-8]
  2,2,6,6-Tetramethyl-2,6-disilaheptane
  Hexamethyldisilylpropane
  Group-member nr.: 71-027

$C_9H_{24}Si_3$
- 1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane [1627-99-2]
  Group-member nr.: 71-028

$C_{10}F_{16}$
- Hexadecafluoro-1,2,3,4,5,6,7,8-octahydronaphthalene [54939-04-7]
  Group-member nr.: 21-030

$C_{10}F_{18}$
- *cis*-Octadecafluorodecahydronaphthalene [60433-11-6]
  cis-Perfluorodecaline
  Group-member nr.: 21-031
- *trans*-Octadecafluorodecahydronaphthalene [60433-12-7]
  trans-Perfluorodecaline
  Group-member nr.: 21-032

$C_{10}H_2O_6$
- 1*H*,3*H*-Benzo[1,2-*c*:4,5-*c*']difuran-1,3,5,7-tetrone [89-32-7]
  1,2,4,5-Benzenetetracarboxylic 1,2:4,5 dianhydride
  Pyromellitic dianhydride
  Group-member nr.: 44-024

$C_{10}H_6O_2S$
- 1-Oxide naphtho[1,8-*cd*]-1,2-dithiole [49833-12-7]
  Naphthalene 1,8-disulfide-*S*-oxide
  Group-member nr.: 63-005

$C_{10}H_7Cl$
- 1-Chloronaphthalene [90-13-1]
  Group-member nr.: 22-044
- 2-Chloronaphthalene [91-58-7]
  Group-member nr.: 22-045

$C_{10}H_7NO_2$
- 1-Nitronaphthalene [86-57-7]
  α-Nitronaphthalene
  Group-member nr.: 62-084

$C_{10}H_8$
- Naphthalene [91-20-3]
  Group-member nr.: 14-033

$C_{10}H_8O$
- 1-Naphthol [90-15-3]
  α-Naphthol
  Group-member nr.: 42-085
- 2-Naphthol [135-19-3]
  β-Naphthol
  Group-member nr.: 42-086

$C_{10}H_9N$
- 2-Naphthalenamine [91-59-8]
  β-Naphthalenamine
  2-Aminonaphthalene
  Group-member nr.: 31-039

$C_{10}H_{10}$
- Tricyclo[3.3.2.$0^{2,8}$]deca-3,6,9-triene [1005-51-2]
  Group-member nr.: 14-034

$C_{10}H_{10}Fe$
- Ferrocene [102-54-5]
  Dicyclopentadienyliron
  Group-member nr.: 73-028

$C_{10}H_{10}O_2$
- 2-Propenyl benzoate [583-04-0]
  2-Propenyl ester benzoic acid
  Allyl benzoate
  Group-member nr.: 45-075

$C_{10}H_{10}O_4$
- Dimethyl 1,2-benzenedicarboxylate [131-11-3]
  Dimethyl phthalate
  Dimethyl ester 1,2-benzenedicarboxylic acid
  Group-member nr.: 45-076
- Dimethyl 1,4-benzenedicarboxylate [120-61-6]
  Dimethyl terephthalate
  Dimethyl ester 1,4-benzenedicarboxylic acid
  Group-member nr.: 45-077

$C_{10}H_{12}$
- 1,2,3,4-Tetrahydronaphthalene [119-64-2]
  Tetralin
  Group-member nr.: 14-035

$C_{10}H_{12}O$
- 1-(4-Ethylphenyl)ethanone [937-30-4]
  4'-Ethylacetophenone
  Group-member nr.: 43-046
- 1-Methoxy-4-(1-propenyl)benzene [104-46-1]
  p-Propenylanisole
  Anethole
  Group-member nr.: 41-041

$C_{10}H_{12}O_2$
- 2-Methoxy-4-(2-propenyl)phenol [97-53-0]
  4-Allyl-2-methoxyphenol
  Eugenol
  Group-member nr.: 47-037
- Propyl benzoate [2315-68-6]
  Propyl ester benzoic acid
  Group-member nr.: 45-078

$C_{10}H_{13}NO_2$
- Propyl ester phenylcarbamic acid [5532-90-1]
  Propyl phenylcarbamate
  Propyl ester carbanilic acid
  Group-member nr.: 62-085

$C_{10}H_{14}$
- Butylbenzene [104-51-8]
  1-Phenylbutane
  Group-member nr.: 14-036
- (1,1-Dimethylethyl)benzene [98-06-6]
  tert-Butylbenzene
  2-Methyl-2-phenylpropane
  Group-member nr.: 14-037
- 1-Methyl-4-(1-methylethyl)benzene [99-87-6]
  1-Isopropyl-4-methylbenzene
  p-Cymene
  Group-member nr.: 14-038
- (1-Methylpropyl)benzene [135-98-8]
  sec-Butylbenzene
  2-Phenylbutane
  Group-member nr.: 14-039
- 1,2,3,4-Tetramethylbenzene [488-23-3]
  Prehnitene
  Group-member nr.: 14-040
- 1,2,3,5-Tetramethylbenzene [527-53-7]
  Isodurene
  Group-member nr.: 14-041
- 1,2,4,5-Tetramethylbenzene [95-93-2]
  Durene
  Group-member nr.: 14-042

$C_{10}H_{14}O$
- 2-Methyl-5-(1-methylethyl)phenol [499-75-2]
  5-Isopropyl-2-methylphenol
  Carvacrol
  Group-member nr.: 42-087

$C_{10}H_{14}O_4$
- Di-2-propenyl butanedioate [925-16-6]
  Di-2-propenyl ester butanedioic acid
  Diallyl succinate
  Group-member nr.: 45-079

$C_{10}H_{14}Si$
- Ethenyldimethylphenylsilane [1125-26-4]
  Group-member nr.: 71-029

$C_{10}H_{15}N$
- *N*, *N*-Diethylbenzenamine [91-66-7]
  N, *N*-Diethylaniline
  Group-member nr.: 31-040

$C_{10}H_{15}NO$
- (*E*)-(±)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one oxime [55658-55-4]
  dl-Carvoxime
  Group-member nr.: 62-086

- [*R*-(*E*)]-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one oxime [60827-56-7]
  l-Carvoxime
  Group-member nr.: 62-087

$C_{10}H_{16}$
- 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane [127-91-3]
  β-Pinene
  Nopinene
  Terebenthene
  Group-member nr.: 12-045
- 4-Methylene-1-(1-methylethyl)bicyclo[3.1.0] - hexane [3387-41-5]
  Sabinene
  Group-member nr.: 12-046
- 1-Methyl-4-(1-methylethenyl)cyclohexene [138-86-3]
  Limonene
  Group-member nr.: 14-043
- Octahydro-4,7-methano-1*H*-indene [6004-38-2]
  Hexahydro-4,7-methanoindan
  Tricyclo[5.2.1.$0^{2,6}$]decane
  Tetrahydrodicyclopentadiene
  Group-member nr.: 12-047

$C_{10}H_{16}O$
- Camphor [76-22-2]
  1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one
  Group-member nr.: 43-047
- 3,7-Dimethyl-2,6-octadienal [5392-40-5]
  Citral
  Group-member nr.: 43-048
- 3,7-Dimethyl-6-octen-1-yn-3-ol [29171-20-8]
  Dehydrolynalol
  Group-member nr.: 42-088
- 5-Methyl-2-(1-methylethylidene)cyclohexanone [15932-80-6]
  p-Menth-4(8)-en-3-one
  1-Isopropylidene-4-methylcyclo-hexan-2-on
  Pulegone
  Group-member nr.: 43-049

$C_{10}H_{18}$
- 1,1'-Bicyclopentyl [1636-39-1]
  Cyclopentylcyclopentane
  Group-member nr.: 12-048
- *cis*-Decahydroazulene [16189-46-1]
  cis-Perhydroazulene
  cis-Bicyclo[5.3.0]decane
  Group-member nr.: 12-049
- Decahydronaphthalene [91-17-8]
  Decalin (unspecified stereoisomer)
  Group-member nr.: 12-050
- *cis*-Decahydronaphthalene [493-01-6]
  cis-Decalin
  Group-member nr.: 12-051
- *trans*-Decahydronaphthalene [493-02-7]
  trans-Decalin
  Group-member nr.: 12-052
- Octahydromethyl-1*H*-indene [unknown]
  Hexahydromethylindan
  Methylhydrindan (unspecified isomer)
  Group-member nr.: 12-053
- 2,6,6-Trimethylbicyclo[3.1.1]heptane [473-55-2]
  Pinane
  Group-member nr.: 12-054

$C_{10}H_{18}O$
- 3,7-Dimethyl-1,6-octadien-3-ol [78-70-6]
  Linalol
  Group-member nr.: 42-089

$C_{10}H_{18}O_4$
- Bis(2-methylpropyl) ethanedioate [2050-61-5]
  Bis(2-methylpropyl) ester ethanedioic acid
  Diisobutyl oxalate
  Group-member nr.: 45-080
- Dipropyl butanedioate [925-15-5]
  Dipropyl ester butanedioic acid
  Dipropyl succinate
  Group-member nr.: 45-081
- 1,2-Ethanediyl dibutanoate [105-72-6]
  1,2-Ethanediyl ester butanoic acid
  1,2-Ethanediol dibutyrate
  Ethylene glycol dibutyrate
  Group-member nr.: 45-082

$C_{10}H_{20}$
- Butylcyclohexane [1678-93-9]
  Group-member nr.: 12-055
- 1-Decene [872-05-9]
  1-Decylene
  α-Decylene
  Group-member nr.: 13-035
- Diethylcyclohexane (unspecified isomer) [1331-43-7]
  Group-member nr.: 12-056
- 1,4-Diethylcyclohexane [1679-00-1]
  Group-member nr.: 12-057
- (1,1-Dimethylethyl)cyclohexane [3178-22-1]
  tert-Butylcyclohexane
  Group-member nr.: 12-058

$C_{10}H_{20}O$
- Decanal [112-31-2]
  Decyl aldehyde
  Capric aldehyde
  Group-member nr.: 43-050

$C_{10}H_{20}O_2$
- Decanoic acid [334-48-5]
  Capric acid
  Group-member nr.: 44-025
- Hexyl butanoate [2639-63-6]
  Hexyl butyrate
  Group-member nr.: 45-083

- 3-Methylbutyl pentanoate [2050-09-1]
  Isoamyl valerate
  Isopentyl valerate
  Group-member nr.: 45-084
- Octyl acetate [112-14-1]
  Group-member nr.: 45-085

$C_{10}H_{20}O_4$
- 2-(2-Butoxyethoxy)ethanol acetate [124-17-4]
  2-(2-Butoxyethoxy)ethyl acetate
  Diethylene glycol butyl ether acetate
  Group-member nr.: 47-038

$C_{10}H_{20}O_5$
- 1,4,7,10,13-Pentaoxacyclopentadecane [33100-27-5]
  Group-member nr.: 46-025

$C_{10}H_{21}NO$
- *N*, *N*-Dibutylacetamide [1563-90-2]
  Group-member nr.: 62-088

$C_{10}H_{22}$
- Decane [124-18-5]
  Decyl hydride
  Group-member nr.: 11-041
- 2,7-Dimethyloctane [1072-16-8]
  Group-member nr.: 11-042
- 2-Methylnonane [871-83-0]
  Isodecane
  Group-member nr.: 11-043
- 3-Methylnonane [5911-04-6]
  Group-member nr.: 11-044
- 4-Methylnonane [17301-94-9]
  Group-member nr.: 11-045
- 5-Methylnonane [15869-85-9]
  Group-member nr.: 11-046

$C_{10}H_{22}N_4$
- 1,1'-(1,2-Ethanediyl)bispiperazine [19479-83-5]
  Dipiperazinylethane
  Group-member nr.: 33-040

$C_{10}H_{22}O$
- 1-Decanol [112-30-1]
  Decyl alcohol
  Group-member nr.: 42-090
- 5-Decanol [5205-34-5]
  Group-member nr.: 42-091
- 3,7-Dimethyl-1-octanol [106-21-8]
  Group-member nr.: 42-092
- 4-Propyl-4-heptanol [2198-72-3]
  Group-member nr.: 42-093

$C_{10}H_{22}O_2$
- 1,1'-[1,2-Ethanediylbis(oxy)]bisbutane [112-48-1]
  1,2-Dibutoxyethane
  Ethylene glycol dibutyl ether
  Group-member nr.: 41-042
- 1,1'-[Ethylidenebis(oxy)]bisbutane [871-22-7]
  1,1-Dibutoxyethane
  Acetaldehyde dibutylacetal
  6-Methyl-5,7-dioxaundecane
  Group-member nr.: 41-043

$C_{10}H_{22}O_5$
- 2,5,8,11,14-Pentaoxapentadecane [143-24-8]
  Bis(methoxyethoxyethyl) ether
  Tetraethylene glycol dimethyl ether
  Group-member nr.: 41-044

$C_{10}H_{22}O_6$
- 3,6,9,12-Tetraoxatetradecane-1,14-diol [4792-15-8]
  Pentaethylene glycol
  Group-member nr.: 47-039

$C_{10}H_{22}S$
- 1-Decanethiol [143-10-2]
  1-Decyl mercaptan
  Group-member nr.: 52-018
- 1,1'-Thiobispentane [872-10-6]
  6-Thiaundecane
  Dipentyl sulfide
  Group-member nr.: 51-022

$C_{10}H_{25}N_5$
- *N*-(2-Aminoethyl)-1,4-piperazinediethanamine [31295-54-2]
  1-(2-Aminoethyl)-4-[2-[(2-aminoethyl)-amino]ethyl]piperazine
  Group-member nr.: 33-041

$C_{10}H_{26}O_3Si_3$
- 2,2,4,4-Tetraethyl-6,6-dimethylcyclotrisiloxane [110505-51-6]
  Group-member nr.: 71-030

$C_{11}H_{10}$
- 1-Methylnaphthalene [90-12-0]
  α-Methylnaphthalene
  Group-member nr.: 14-044
- 2-Methylnaphthalene [91-57-6]
  β-Methylnaphthalene
  Group-member nr.: 14-045

$C_{11}H_{12}O_2$
- Ethyl 3-phenyl-2-propenoate [103-36-6]
  Ethyl ester 3-phenyl-2-propenoic acid
  Ethyl cinnamate (unspecified stereoisomer)
  Group-member nr.: 45-086
- Phenylmethyl 2-methyl-2-propenoate [2495-37-6]
  Phenylmethyl ester 2-methyl-2-propenoic acid
  Benzyl methacrylate
  Group-member nr.: 45-087

$C_{11}H_{14}$
- 1,1-Dimethylindan [4912-92-9]
  Group-member nr.: 14-046

- 4,6-Dimethylindan [1685-82-1]
  Group-member nr.: 14-047
- 4,7-Dimethylindan [6682-71-9]
  Group-member nr.: 14-048

$C_{11}H_{14}O_2$
- Ethyl benzenepropanoate [2021-28-5]
  Ethyl ester benzenepropanoic acid
  Ethyl 3-phenylpropanoate
  Ethyl hydrocinnamate
  Group-member nr.: 45-088

$C_{11}H_{16}$
- Pentamethylbenzene [700-12-9]
  Group-member nr.: 14-049

$C_{11}H_{16}Si$
- Ethenyldimethyl(phenylmethyl)silane [18001-46-2]
  Benzyldimethylvinylsilane
  Group-member nr.: 71-031

$C_{11}H_{20}$
- Decahydro-1-methylnaphthalene [2958-75-0]
  α-Methyldecalin
  Group-member nr.: 12-059
- Decahydro-2-methylnaphthalene [2958-76-1]
  β-Methyldecalin
  Group-member nr.: 12-060
- Ethyloctahydro-1*H*-indene [95098-51-4]
  Ethylhexahydroindan
  Ethylhydrindan (unspecified isomer)
  Group-member nr.: 12-061

$C_{11}H_{20}O_2$
- Oxacyclododecan-2-one [1725-03-7]
  Undecanolide
  Undecanolactone
  Group-member nr.: 47-040

$C_{11}H_{22}$
- 1-Undecene [821-95-4]
  α-Undecene
  Group-member nr.: 13-036

$C_{11}H_{22}O_2$
- Methyl decanoate [110-42-9]
  Methyl caprate
  Group-member nr.: 45-089
- Undecanoic acid [112-37-8]
  Undecylic acid
  Group-member nr.: 44-026

$C_{11}H_{24}$
- 2-Methyldecane [6975-98-0]
  Group-member nr.: 11-047
- Undecane [1120-21-4]
  Hendecane
  Group-member nr.: 11-048

$C_{11}H_{24}O$
- 1-Methoxydecane [7289-52-3]
  Decyl methyl ether
  Group-member nr.: 41-045
- 1-Undecanol [112-42-5]
  Undecyl alcohol
  Decyl carbinol
  1-Hendecanol
  Group-member nr.: 42-094

$C_{12}F_{10}$
- 2,2',3,3',4,4',5,5',6,6'-Decafluoro-1,1'-biphenyl [434-90-2]
  Decafluorobiphenyl
  Perfluorobiphenyl
  Group-member nr.: 21-033

$C_{12}H_8$
- Acenaphthylene [208-96-8]
  Group-member nr.: 14-050

$C_{12}H_8Cl_2O_2S$
- 1,1'-Sulfonylbis(4-chlorobenzene) [80-07-9]
  Bis(*p*-chlorophenyl)sulfone
  4,4'-Dichlorodiphenyl sulfone
  Group-member nr.: 64-027

$C_{12}H_8N_2O_5$
- 1,1'-Oxybis(4-nitrobenzene) [101-63-3]
  Bis(*p*-nitrophenyl) ether
  4,4'-Dinitrodiphenyl ether
  Group-member nr.: 62-089

$C_{12}H_8O$
- Dibenzofuran [132-64-9]
  Diphenylene oxide
  Group-member nr.: 46-026

$C_{12}H_8OS_2$
- Dibenzo[*c,e*][1,2]dithiin-5-oxide [49833-13-8]
  Diphenylene 2,2'-disulfide-*S*-oxide
  Group-member nr.: 63-006

$C_{12}H_8S$
- Dibenzothiophene [132-65-0]
  Group-member nr.: 53-013

$C_{12}H_9Cl$
- 2-Chloro-1,1'-biphenyl [2051-60-7]
  o-Chlorobiphenyl
  o-Chlorodiphenyl
  Group-member nr.: 22-046
- 4-Chloro-1,1'-biphenyl [2051-62-9]
  p-Chlorobiphenyl
  p-Chlorodiphenyl
  Group-member nr.: 22-047

$C_{12}H_9Cl_3Si$
- [1,1'-Biphenyl]-2-yltrichlorosilane [18030-62-1]
  o-(Trichlorosilyl)biphenyl
  o-Trichlorosilanediphenyl
  Group-member nr.: 71-032
- [1,1'-Biphenyl]-4-yltrichlorosilane [18030-61-0]
  p-(Trichlorosilyl)biphenyl
  p-Trichlorosilanediphenyl
  Group-member nr.: 71-033

$C_{12}H_{10}$
- Acenaphthene [83-32-9]
  1,8-Dihydroacenaphthalene
  Ethylenenaphthalene
  Group-member nr.: 14-051
- 1,1'-Biphenyl [92-52-4]
  Diphenyl
  Group-member nr.: 14-052

$C_{12}H_{10}N_2$
- Diphenyldiazene [103-33-3]
  Azobenzene
  Diphenyldiimide (unspecified stereoisomer)
  Group-member nr.: 34-011
- (*E*)-Diphenyldiazene [17082-12-1]
  trans-Azobenzene
  trans-Diphenyldiimide
  Group-member nr.: 34-012

$C_{12}H_{10}O$
- 1,1'-Oxybisbenzene [101-84-8]
  Diphenyl ether
  Diphenyl oxide
  Group-member nr.: 41-046

$C_{12}H_{10}S$
- 1,1'-Thiobisbenzene [139-66-2]
  Diphenyl sulfide
  Phenyl sulfide
  Group-member nr.: 51-023

$C_{12}H_{11}N$
- [1,1'-Biphenyl]-2-amine [90-41-5]
  2-Aminobiphenyl
  Group-member nr.: 31-041
- *N*-Phenylbenzenamine [122-39-4]
  Diphenylamine
  Group-member nr.: 31-042

$C_{12}H_{12}$
- 1,8-Dimethylnaphthalene [569-41-5]
  Group-member nr.: 14-053
- 2,3-Dimethylnaphthalene [581-40-8]
  Group-member nr.: 14-054
- 2,6-Dimethylnaphthalene [581-42-0]
  Group-member nr.: 14-055
- 2,7-Dimethylnaphthalene [582-16-1]
  Group-member nr.: 14-056

$C_{12}H_{12}Ge$
- Diphenylgermane [1675-58-7]
  Group-member nr.: 73-029

$C_{12}H_{12}N_2O$
- 4,4'-Oxybisbenzenamine [101-80-4]
  4,4'-Oxydianiline
  4,4'-Diaminodiphenyl ether
  Group-member nr.: 62-090

$C_{12}H_{12}N_2O_2S$
- 4,4'-Sulfonylbisbenzenamine [80-08-0]
  4,4'-Sulfonyldianiline
  4-Aminophenyl sulfone
  Dapsone
  Group-member nr.: 64-028

$C_{12}H_{14}O_4$
- Diethyl 1,2-benzenedicarboxylate [84-66-2]
  Diethyl phthalate
  Diethyl ester
  1,2-benzenedicarboxylic acid
  Group-member nr.: 45-090
- Diethyl 1,4-benzenedicarboxylate [636-09-9]
  Diethyl terephthalate
  Diethyl ester 1,4-benzenedicarboxylic acid
  Group-member nr.: 45-091

$C_{12}H_{16}$
- Cyclohexylbenzene [827-52-1]
  Phenylcyclohexane
  Group-member nr.: 14-057

$C_{12}H_{18}$
- (*E*, *E*, *Z*)-1,5,9-Cyclododecatriene [706-31-0]
  trans,trans,cis-1,5,9-Cyclododecatriene
  Group-member nr.: 14-058
- Decahydrodimethanonaphthalene [unknown]
  Dimethanodecalin (unspecified isomer)
  Group-member nr.: 12-062
- Hexamethylbenzene [87-85-4]
  Mellitene
  Group-member nr.: 14-059
- Hexylbenzene [1077-16-3]
  1-Phenylhexane
  Group-member nr.: 14-060

$C_{12}H_{20}$
- 1,3-Dimethyltricyclo[3.3.1.$1^{3,7}$]decane [702-79-4]
  1,3-Dimethyladamantane
  Group-member nr.: 12-063
- Tricyclo[6.2.1.$1^{3,6}$]dodecane [281-84-5]
  Group-member nr.: 12-064

$C_{12}H_{20}O_6$
- 1,2,3-Propanetriyl tripropanoate [139-45-7]
  1,2,3-Propanetriyl ester propanoic acid
  Tripropionin
  Group-member nr.: 45-092

$C_{12}H_{22}$
- 1,1'-Bicyclohexyl [92-51-3]
  Cyclohexylcyclohexane
  Dodecahydrobiphenol
  Group-member nr.: 12-065
- Decahydrodimethylnaphthalene [28777-88-0]
  Dimethyldecalin (unspecified isomer)
  Group-member nr.: 12-066
- Ethyldecahydronaphthalene [25551-49-9]
  Ethyldecalin (unspecified isomer)
  Group-member nr.: 12-067
- 1-Ethyldecahydronaphthalene [1008-17-9]
  1-Ethyldecalin
  α-Ethyldecalin (unspecified stereoisomer)
  Group-member nr.: 12-068
- 2-Ethyldecahydronaphthalene [1618-23-1]
  2-Ethyldecalin
  β-Ethyldecalin (unspecified stereoisomer)
  Group-member nr.: 12-069
- Octahydro(1-methylethyl)-1*H*-indene [88889-26-3]
  Hexahydroisopropylindan
  Isopropylhydrindan (unspecified isomer)
  Group-member nr.: 12-070

$C_{12}H_{22}O_2$
- Nonyl 2-propenoate [2664-55-3]
  Nonyl ester 2-propenoic acid
  Nonyl acrylate
  Group-member nr.: 45-093
- Octyl 2-methyl-2-propenoate [2157-01-9]
  Octyl ester 2-methyl-2-propenoic acid
  Octyl methacrylate
  Group-member nr.: 45-094

$C_{12}H_{22}O_4$
- Bis(3-methylbutyl) ethanedioate [2051-00-5]
  Bis(3-methylbutyl) ester ethanedioic acid
  Diisoamyl oxalate
  Group-member nr.: 45-095
- Bis(2-methylpropyl) butanedioate [925-06-4]
  Bis(2-methylpropyl) ester butanedioic acid
  Diisobutyl succinate
  Group-member nr.: 45-096
- Dibutyl butanedioate [141-03-7]
  Dibutyl ester butanedioic acid
  Dibutyl succinate
  Group-member nr.: 45-097

$C_{12}H_{22}O_4Pb$
- Lead(2+) salt hexanoic acid [15773-53-2]
  Lead(II) hexanoate
  Lead(II) caproate
  Group-member nr.: 74-004

$C_{12}H_{24}$
- 1-Dodecene [112-41-4]
  α-Dodecylene
  Group-member nr.: 13-037

$C_{12}H_{24}N_2O_2$
- *N*, *N*'-Dipropylhexanediamine [10263-96-4]
  N, *N*'-Dipropyladipamide
  Group-member nr.: 62-091

$C_{12}H_{24}O_2$
- Decyl acetate [112-17-4]
  Group-member nr.: 45-098
- Dodecanoic acid [143-07-7]
  Lauric acid
  Group-member nr.: 44-027

$C_{12}H_{25}NO$
- *N*, *N*-Dipentylacetamide [16238-16-7]
  Group-member nr.: 62-092

$C_{12}H_{26}$
- Dodecane [112-40-3]
  Dihexyl
  Group-member nr.: 11-049
- 2,2,4,6,6-Pentamethylheptane [13475-82-6]
  Group-member nr.: 11-050

$C_{12}H_{26}O$
- 1-Dodecanol [112-53-8]
  Dodecyl alcohol
  Lauryl alcohol
  Group-member nr.: 42-095

$C_{12}H_{26}O_3$
- 1,1'-[Oxybis(2,1-ethanediyloxy)]bisbutane [112-73-2]
  Bis(2-butoxyethyl)ether
  Diethylene glycol dibutyl ether
  Group-member nr.: 41-047

$C_{12}H_{26}S$
- 1,1'-Thiobishexane [6294-31-1]
  7-Thiatridecane
  Dihexyl sulfide
  Group-member nr.: 51-024

$C_{12}H_{28}O_4Si$
- Tetrapropyl ester silicic acid [682-01-9]
  Tetrapropyl orthosilicate
  Tetrapropoxysilane
  Group-member nr.: 71-034

$C_{12}H_{30}OSi_2$
- Hexaethyldisiloxane [994-49-0]
  Group-member nr.: 71-035

$C_{12}H_{30}O_3Si_3$
- Hexaethylcyclotrisiloxane [2031-79-0]
  Group-member nr.: 71-036

$C_{13}H_9N$
- Acridine [260-94-6]
  Benzo[*b*]quinoline
  2,3,5,6-Dibenzopyridine
  Group-member nr.: 33-042
- Benzo[*h*]quinoline [230-27-3]
  7,8-Benzoquinoline
  Group-member nr.: 33-043
- Phenanthridine [229-87-8]
  Benzo[c]quinoline
  Group-member nr.: 33-044

$C_{13}H_{10}$
- 9*H*-Fluorene [86-73-7]
  α-Diphenylenemethane
  Group-member nr.: 14-061

$C_{13}H_{10}N_2$
- *N*, *N*'-Methanetetraylbisbenzenamine [622-16-2]
  Diphenylcarbodiimide
  Group-member nr.: 34-013

$C_{13}H_{10}O$
- Diphenyl methanone [119-61-9]
  Diphenyl ketone
  Benzophenone
  Group-member nr.: 43-051

$C_{13}H_{10}O_3$
- Phenyl ester 2-hydroxybenzoic acid [118-55-8]
  Phenyl salicylate
  Salol
  Group-member nr.: 47-041

$C_{13}H_{11}Cl$
- 1,1'-(Chloromethylene)bisbenzene [90-99-3]
  Diphenylchloromethane
  Group-member nr.: 22-048

$C_{13}H_{11}N$
- 9-Methyl-9*H*-carbazole [1484-12-4]
  Group-member nr.: 33-045

$C_{13}H_{12}$
- 1,1'-Methylenebisbenzene [101-81-5]
  Diphenylmethane
  Benzylbenzene
  Group-member nr.: 14-062

$C_{13}H_{13}N$
- *N*-Methyl-*N*-phenylbenzenamine [552-82-9]
  N-Methyldiphenylamine
  Group-member nr.: 31-043

$C_{13}H_{14}N_2$
- 4,4'-Methylenebisbenzenamine [101-77-9]
  4,4'-Methylenedianiline
  Bis-(4-aminophenyl)methane
  Group-member nr.: 31-044

$C_{13}H_{15}N$
- 2,3,4,9-Tetrahydro-9-methyl-1*H*-carbazole [6303-88-4]
  1,2,3,4-Tetrahydro-9-methylcarbazole
  Group-member nr.: 33-046

$C_{13}H_{15}NO$
- 1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl) benzene [2094-99-7]
  m-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid
  Group-member nr.: 62-093
- 1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl) benzene [2889-58-9]
  p-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid
  Group-member nr.: 62-094

$C_{13}H_{18}$
- 1,1,4,6-Tetramethylindan [941-60-6]
  Group-member nr.: 14-063
- 1,1,4,7-Tetramethylindan [1078-04-2]
  Group-member nr.: 14-064

$C_{13}H_{19}NO_2$
- Hexyl ester phenylcarbamic acid [7461-26-9]
  Hexyl phenylcarbamate
  Hexyl ester carbanilic acid
  Group-member nr.: 62-095

$C_{13}H_{20}$
- Heptylbenzene [1078-71-3]
  1-Phenylheptane
  Group-member nr.: 14-065

$C_{13}H_{20}O$
- 6,10-Dimethyl-3,5,9-undecatriene-2-one [141-10-6]
  Pseudoionone
  ψ-Ionone
  Group-member nr.: 43-052
- 6,10-Dimethyl-4,5,9-undecatriene-2-one [16647-05-5]
  Group-member nr.: 43-053
- 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one [14901-07-6]
  β-Ionone
  Group-member nr.: 43-054

$C_{13}H_{22}$
- 1,3,5-Trimethyltricyclo[3.3.1.$1^{3,7}$]decane [707-35-7]
  1,3,5-Trimethyladamantane
  Group-member nr.: 12-071

$C_{13}H_{24}$
- Decahydro(1-methylethyl)naphthalene [27193-29-9]
  Isopropyldecalin (unspecified isomer)
  Group-member nr.: 12-072
- Decahydro-1-(1-methylethyl)naphthalene [1010-74-8]
  Decahydro-1-isopropylnaphthalene
  α-Isopropyldecalin
  Group-member nr.: 12-073

- Decahydro-1-propylnaphthalene [91972-45-1]
  1-Propyldecalin
  α-Propyldecalin
  Group-member nr.: 12-074
- 2-Methyl-1,1'-bicyclohexyl [unknown]
  1-Methylcyclohexylcyclohexane
  Group-member nr.: 12-075
- 1,1'-Methylenebiscyclohexane [3178-23-2]
  Dicyclohexylmethane
  Group-member nr.: 12-076

$C_{13}H_{24}O_2$
- Nonyl 2-methyl-2-propenoate [2696-43-7]
  Nonyl ester 2-methyl-2-propenoic acid
  Nonyl methacrylate
  Group-member nr.: 45-099
- Oxacyclotetradecan-2-one [1725-04-8]
  Tridecanolide
  Tridecanolactone
  Group-member nr.: 47-042

$C_{13}H_{26}$
- Heptylcyclohexane [5617-41-4]
  Group-member nr.: 12-077

$C_{13}H_{26}O$
- 6,10-Dimethyl-2-undecanone [1604-34-8]
  Hexahydropseudoionone
  Group-member nr.: 43-055

$C_{13}H_{26}O_2$
- Tridecanoic acid [638-53-9]
  Tridecylic acid
  Group-member nr.: 44-028

$C_{13}H_{26}O_2Si_3$
- 1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane [546-44-1]
  Group-member nr.: 71-037

$C_{13}H_{28}$
- Tridecane [629-50-5]
  Group-member nr.: 11-051

$C_{13}H_{28}O$
- 5-Butyl-5-nonanol [597-93-3]
  Group-member nr.: 42-096
- 1-Tridecanol [112-70-9]
  n-Tridecyl alcohol
  Group-member nr.: 42-097

$C_{14}H_8O_2$
- 9,10-Anthracenedione [84-65-1]
  9,10-Antraquinone
  Group-member nr.: 43-056

$C_{14}H_{10}$
- Anthracene [120-12-7]
  Group-member nr.: 14-066
- 1,1'-(1,2-Ethynediyl)bisbenzene [501-65-5]
  1,2-Diphenylacetylene
  Tolan
  Group-member nr.: 14-067
- Phenanthrene [85-01-8]
  Group-member nr.: 14-068

$C_{14}H_{12}$
- (*E*)-1,1'-(1,2-Ethenediyl)bisbenzene [103-30-0]
  trans-1,2-Diphenylethylene
  Stilbene
  Toluylene
  Group-member nr.: 14-070
- 9,10-Dihydrophenanthrene [776-35-2]
  Group-member nr.: 14-069
- 1,1'-Ethenylidenebisbenzene [530-48-3]
  1,1-Diphenylethylene
  Group-member nr.: 14-071

$C_{14}H_{12}O$
- (3-Methylphenyl)phenylmethanone [643-65-2]
  3-Methylbenzophenone
  Phenyl *m*-tolyl ketone
  Group-member nr.: 43-057

$C_{14}H_{14}$
- 1,1'-(1,2-Ethanediyl)bisbenzene [103-29-7]
  Bibenzyl
  1,2-Diphenylethane
  sym-Diphenylethane
  Dibenzyl
  Group-member nr.: 14-072
- 1,1'-Ethylidenebisbenzene [612-00-0]
  1,1-Diphenylethane
  unsym-Diphenylethane
  Group-member nr.: 14-073

$C_{14}H_{14}N_2O_3$
- Bis(4-methoxyphenyl)diazene-1-oxide [1562-94-3]
  4,4'-Dimethoxyazoxybenzene
  p-Azoxyanisole
  Group-member nr.: 62-096

$C_{14}H_{16}N_2O_2$
- 1,3-Bis(1-isocyanato-1-methylethyl)benzene [2778-42-9]
  α,α,α',α'-Tetramethyl-*m*-xylylene ester isocyanic acid
  Group-member nr.: 62-097
- 1,4-Bis(1-isocyanato-1-methylethyl)benzene [2778-41-8]
  α,α,α',α'-Tetramethyl-*p*-xylylene ester isocyanic acid
  Group-member nr.: 62-098

$C_{14}H_{18}$
- 1,2,3,4,5,6,7,8-Octahydroanthracene [1079-71-6]
  Group-member nr.: 14-074

$C_{14}H_{20}$
- Decahydro-3,5,1,7-[1,2,3,4]butanetetraylnaphthalene [2292-79-7]
  Diamantane
  Group-member nr.: 12-078

$C_{14}H_{20}O_3$
- 1-[4-(1,1-Diethoxyethyl)phenyl]ethanone [64533-95-5]
  p-Diacetylbenzene diethyl ketal
  Group-member nr.: 47-043

$C_{14}H_{22}$
- Octylbenzene [2189-60-8]
  1-Phenyloctane
  Group-member nr.: 14-075

$C_{14}H_{24}$
- Dodecahydro-9-methylfluorene [92431-75-9]
  9-Methylperhydrofluorene
  Group-member nr.: 12-079
- Tetradecahydrophenanthrene [5743-97-5]
  Perhydrophenanthrene (unspecified stereoisomer)
  Group-member nr.: 12-080
- (4aα,4bα,8aα,10aβ)-Tetradecahydrophenanthrene [27425-35-0]
  cis-syn-trans-Perhydrophenantrene
  Group-member nr.: 12-081
- (4aα,4bβ,8aα,10aα)-Tetradecahydrophenanthrene [27389-73-7]
  trans-anti-cis-Perhydrophenanthrene
  Group-member nr.: 12-082
- (4aα,4bβ,8aα,10aβ)-Tetradecahydrophenanthrene [2108-89-6]
  trans-anti-trans-Perhydrophenanthrene
  Group-member nr.: 12-083

$C_{14}H_{26}$
- 1-Butyldecahydronaphthalene [92369-80-7]
  1-Butyldecalin
  α-Butyldecalin
  Group-member nr.: 12-084
- 1-(Cyclohexylmethyl)-2-methylcyclohexane [66826-96-8]
  Cyclohexyl(2-methylcyclohexyl)methane
  Group-member nr.: 12-085
- Decahydro-1-(1-methylpropyl)naphthalene [92369-82-9]
  1-*sec*-Butyldecahydronaphthalene
  α-*sec*-Butyldecalin
  Group-member nr.: 12-086
- Decahydro-1-(2-methylpropyl)naphthalene [92369-83-0]
  Decahydro-1-isobutylnaphthalene
  α-Isobutyldecalin
  Group-member nr.: 12-087
- (1,1-Dimethylethyl)decahydronaphthalene [27193-30-2]
  tert-Butyldecalin (unspecified isomer)
  Group-member nr.: 12-088
- 1,1'-(1,2-Ethanediyl)biscyclohexane [3321-50-4]
  1,2-Dicyclohexylethane
  Group-member nr.: 12-089
- 2-Ethyl-1,1'-bicyclohexyl [66826-94-6]
  2-Ethylcyclohexylcyclohexane
  Group-member nr.: 12-090
- 1,1'-Ethylidenebiscyclohexane [2319-61-1]
  1,1-Dicyclohexylethane
  Group-member nr.: 12-091

$C_{14}H_{26}O$
- 2-(1,2-Dimethylpropyl)-5,6-dimethyl-2-heptenal [99914-84-8]
  Group-member nr.: 43-058
- 2-Pentyl-2-nonenal [3021-89-4]
  Group-member nr.: 43-059

$C_{14}H_{26}O_2$
- Decyl 2-methyl-2-propenoate [3179-47-3]
  Decyl ester 2-methyl-2-propenoic acid
  Decyl methacrylate
  Group-member nr.: 45-100

$C_{14}H_{26}O_4$
- Bis(3-methylbutyl) butanedioate [818-04-2]
  Bis(3-methylbutyl) ester butanedioic acid
  Diisoamyl succinate
  Group-member nr.: 45-101

$C_{14}H_{28}O$
- 2-Tetradecanone [2345-27-9]
  Dodecyl methyl ketone
  Group-member nr.: 43-060

$C_{14}H_{28}O_2$
- Tetradecanoic acid [544-63-8]
  Myristic acid
  Group-member nr.: 44-029

$C_{14}H_{30}$
- Tetradecane [629-59-4]
  Group-member nr.: 11-052

$C_{14}H_{30}O$
- 1-Tetradecanol [112-72-1]
  n-Tetradecyl alcohol
  Myristyl alcohol
  Group-member nr.: 42-098

$C_{14}H_{30}S$
- 1,1'-Thiobisheptane [629-65-2]
  8-Thiapentadecane
  Diheptyl sulfide
  Group-member nr.: 51-025

$C_{15}H_{10}N_2O_2$
- 1,1'-Methylenebis[4-isocyanatobenzene] [101-68-8]
  Methylenedi-*p*-phenylene ester isocyanic acid
  Diphenylmethane-4,4'-diisocyanate
  Group-member nr.: 62-099

$C_{15}H_{12}$
- 4-Methylphenanthrene [832-64-4]
  Group-member nr.: 14-076

$C_{15}H_{16}$
- (1-Methylethyl)-1,1'-biphenyl [25640-78-2]
  Isopropylbiphenyl
  Isopropyldiphenyl (unspecified isomer)
  Group-member nr.: 14-077

$C_{15}H_{16}N_2O_3$
- (4-Ethoxyphenyl)(4-methoxyphenyl)diazene-*N*-oxide [56095-14-8]
  4-Ethoxy-4'-methoxyazoxybenzene
  p-Azoxyanisoyl-phenetole
  Group-member nr.: 62-100

$C_{15}H_{16}O_2$
- 4,4'-(1-Methylethylidene)bisphenol [80-05-7]
  4,4'-Isopropylidenediphenol
  4,4'-Dihydroxydiphenyl-2,2-propane
  Group-member nr.: 42-099

$C_{15}H_{26}$
- 1,1':3',1''-Tercyclopentane [6051-40-7]
  1,3-Dicyclopentylcyclopentane
  Group-member nr.: 12-092

$C_{15}H_{26}O_6$
- 1,2,3-Propanetriyl tributanoate [60-01-5]
  1,2,3-Propanetriyl ester butanoic acid
  Tributyrin
  Group-member nr.: 45-102

$C_{15}H_{28}$
- Cyclohexyl(ethylcyclohexyl)methane (unspecified isomer) [97239-02-6]
  Group-member nr.: 12-093
- 1-(Cyclohexylmethyl)-2-ethylcyclohexane [66374-71-8]
  Cyclohexyl(2-ethylcyclohexyl)methane
  Group-member nr.: 12-094
- 1,2-Dicyclohexylpropane [41851-34-7]
  Group-member nr.: 12-095
- (1-Methylethyl)-1,1'-bicyclohexyl [31624-59-6]
  Isopropylbicyclohexyl
  Isopropylcyclohexylcyclohexane (unspecified isomer and stereoisomer)
  Group-member nr.: 12-096

$C_{15}H_{28}O$
- 3,7,11-Trimethyl-1-dodecyn-3-ol [1604-35-9]
  Group-member nr.: 42-100

$C_{15}H_{28}O_2$
- Oxacyclohexadecan-2-one [106-02-5]
  Pentadecanolide
  Pentadecanolactone
  15-Hydroxypentadecanoic acid lactone
  Group-member nr.: 47-044

$C_{15}H_{30}$
- Decylcyclopentane [1795-21-7]
  Cyclopentyldecane
  Group-member nr.: 12-097

$C_{15}H_{30}O$
- 2-Pentadecanone [2345-28-0]
  Methyl tridecyl ketone
  Group-member nr.: 43-061

$C_{15}H_{30}O_2$
- Methyl tetradecanoate [124-10-7]
  Methyl myristate
  Group-member nr.: 45-103
- Pentadecanoic acid [1002-84-2]
  Pentadecylic acid
  Group-member nr.: 44-030

$C_{15}H_{32}$
- Pentadecane [629-62-9]
  Group-member nr.: 11-053

$C_{15}H_{32}O$
- 1-Pentadecanol [629-76-5]
  n-Pentadecyl alcohol
  Group-member nr.: 42-101

$C_{16}H_{10}$
- Fluoranthene [206-44-0]
  Group-member nr.: 14-078
- Pyrene [129-00-0]
  Group-member nr.: 14-079

$C_{16}H_{12}Ge$
- Diethynyldiphenylgermane [1675-59-8]
  Group-member nr.: 73-030

$C_{16}H_{12}Si$
- Diethynyldiphenylsilane [1675-57-6]
  Group-member nr.: 71-038

$C_{16}H_{14}O_2$
- 1,4-Diphenyl-1,4-butanedione [495-71-6]
  1,2-Dibenzoylethane
  Group-member nr.: 43-062

$C_{16}H_{16}N_2O_2$
- [(4-Methoxyphenyl)methylene]hydrazone-4-methoxybenzaldehyde [2299-73-2]
  p-Anisaldehydeazine
  Anisaldazine
  Group-member nr.: 62-101

$C_{16}H_{18}N_2O_3$
- Bis(4-ethoxyphenyl)diazene-1-oxide [4792-83-0]
  4,4'-Diethoxyazoxybenzene
  p-Azoxyphenetole
  Group-member nr.: 62-102

$C_{16}H_{22}OSi_2$
- 1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane [56-33-7]
  Group-member nr.: 71-039

$C_{16}H_{22}O_3Si_3$
- 2,2,4,4-Tetramethyl-6,6-diphenylcyclotrisiloxane [1693-51-2]
  Group-member nr.: 71-040

$C_{16}H_{22}O_4$
- Dibutyl 1,2-benzenedicarboxylate [84-74-2]
  Dibutyl ester 1,2-benzenedicarboxylic acid
  Dibutyl phthalate
  Group-member nr.: 45-104

$C_{16}H_{25}NO_2$
- Nonyl phenylcarbamate [33689-71-3]
  Nonyl ester phenylcarbamic acid
  Nonyl ester carbanilic acid
  Group-member nr.: 62-103

$C_{16}H_{28}$
- 1-Cyclohexyloctahydro-3-methyl-1*H*-indene [unknown]
  1-Cyclohexyl-3-methylhydrindan
  Group-member nr.: 12-098
- 2-Ethyltetradecahydrophenanthrene [90591-84-7]
  2-Ethylperhydrophenanthrene
  Group-member nr.: 12-099

$C_{16}H_{30}$
- Cyclohexyl[(1-methylethyl)cyclohexyl]methane [97676-41-0]
  Cyclohexyl(isopropylcyclohexyl)methane (unspecified isomer)
  Group-member nr.: 12-101
- 1,1'-(1-Methyl-1,3-propanediyl)biscyclohexane [41851-35-8]
  1,3-Dicyclohexylbutane
  Group-member nr.: 12-100

$C_{16}H_{30}HgO_4$
- Mercury(2+) salt octanoic acid [28043-54-1]
  Mercury(II) octanoate
  Mercury(II) caprylate
  Group-member nr.: 74-005

$C_{16}H_{30}O_4Pb$
- Lead(2+) salt octanoic acid [7319-86-0]
  Lead(II) octanoate
  Lead(II) caprylate
  Group-member nr.: 74-006

$C_{16}H_{32}$
- Decylcyclohexane [1795-16-0]
  Cyclohexyldecane
  Group-member nr.: 12-102
- 1-Hexadecene [629-73-2]
  α-Hexadecylene
  Cetene
  Group-member nr.: 13-038

$C_{16}H_{32}O_2$
- Hexadecanoic acid [57-10-3]
  Palmitic acid
  Group-member nr.: 44-031

$C_{16}H_{34}$
- 2,2,4,4,6,8,8-Heptamethylnonane [4390-04-9]
  Group-member nr.: 11-054
- Hexadecane [544-76-3]
  Cetane
  Group-member nr.: 11-055

$C_{16}H_{34}O$
- 1-Hexadecanol [36653-82-4]
  Hexadecyl alcohol
  Cetyl alcohol
  Group-member nr.: 42-102

$C_{16}H_{34}S$
- 1,1'-Thiobisoctane [2690-08-6]
  9-Thiaheptadecane
  Dioctyl sulfide
  Group-member nr.: 51-026

$C_{16}H_{35}N$
- *N*, *N*-Dimethyl-2-pentyl-1-nonanamine [99916-30-0]
  N, *N*-Dimethyl-2-pentylnonylamine
  Group-member nr.: 31-045

$C_{16}H_{36}Ge$
- Tetrabutylgermane [1067-42-1]
  Group-member nr.: 73-031

$C_{16}H_{36}O_4Si$
- Tetrabutyl ester silicic acid [4766-57-8]
  Tetrabutyl orthosilicate
  Tetrabutoxysilane
  Group-member nr.: 71-041

$C_{16}H_{36}O_4Ti$
- Titanium(4+) salt 1-butanol [5593-70-4]
  Tetrabutoxytitanium
  Group-member nr.: 74-007

$C_{16}H_{40}O_4Si_4$
- Octaethylcyclotetrasiloxane [1451-99-6]
  Group-member nr.: 71-042

$C_{17}H_{17}NSi$
- 1-[2-(Trimethylsilyl)ethyl]aziridine [18387-12-7]
  N-[(β-Trimethylsilyl)ethyl]ethylenimine
  Group-member nr.: 71-043

$C_{17}H_{30}$
- Cyclopentylbicyclohexyl (unspecified isomer) [26447-22-3]
  Group-member nr.: 12-103

$C_{17}H_{32}$
- Bis(ethylcyclohexyl)methane (unspecified isomer) [98028-64-9]
  Group-member nr.: 12-104
- 1-Cyclohexyl-1-(1-methylethyl)cyclohexylethane [26637-18-3]
  1-Cyclohexyl-1-(isopropylcyclohexyl)ethane (unspecified isomer)
  Group-member nr.: 12-105

$C_{17}H_{34}O_2$
- Heptadecanoic acid [506-12-7]
  Margaric acid
  Group-member nr.: 44-032

$C_{17}H_{36}$
- Heptadecane [629-78-7]
  Group-member nr.: 11-056

$C_{18}H_{12}$
- Triphenylene [217-59-4]
  9,10-Benzophenanthrene
  Group-member nr.: 14-080

$C_{18}H_{14}$
- 1,1':2',1''-Terphenyl [84-15-1]
  o-Terphenyl
  Group-member nr.: 14-081
- 1,1':3',1''-Terphenyl [92-06-8]
  m-Terphenyl
  Group-member nr.: 14-082
- 1,1':4',1''-Terphenyl [92-94-4]
  p-Terphenyl
  Group-member nr.: 14-083

$C_{18}H_{15}ClSi$
- Chlorotriphenylsilane [76-86-8]
  Group-member nr.: 71-044

$C_{18}H_{15}OP$
- Triphenylphosphine oxide [791-28-6]
  Oxotriphenylphosphorane
  Oxotriphenylphosphorus
  Group-member nr.: 72-012

$C_{18}H_{15}O_4P$
- Triphenyl ester phosphoric acid [115-86-6]
  Triphenyl phosphate
  Group-member nr.: 72-013

$C_{18}H_{18}$
- 1-Methyl-7-(1-methylethyl)phenanthrene [483-65-8]
  7-Isopropyl-1-methylphenanthrene
  Retene
  Group-member nr.: 14-084

$C_{18}H_{18}N_2O_5$
- Diethyl ester 4,4'-azoxybisbenzoic acid [6421-04-1]
  Diethyl 4,4'-azoxybisbenzoate
  Ethyl-*p*,*p*-azoxybenzoate
  Group-member nr.: 62-104

$C_{18}H_{21}NO$
- 4-Butyl-*N*-[(4-methoxyphenyl)methylene]-benzenamine [26227-73-6]
  N-(*p*-Methoxybenzylidene)-*p*-butylaniline
  MBBA
  Group-member nr.: 62-105

$C_{18}H_{21}NO_2$
- 2-[[(4-Butylphenyl)imino]methyl]-4-methoxyphenol [52218-22-1]
  N-(*o*-Hydroxy-*p*-methoxybenzylidene)-*p*-butylaniline
  2,4-OHMBBA
  Group-member nr.: 62-106

$C_{18}H_{22}$
- *ar*,*ar*'-Bis(1-methylethyl)-1,1'-biphenyl [36876-13-8]
  Diisopropylbiphenyl (unspecified isomer)
  Group-member nr.: 14-085

$C_{18}H_{22}N_2O$
- (*E*)-(4-Butylphenyl)(4-ethoxyphenyl)diazene [98644-12-3]
  Group-member nr.: 62-107

$C_{18}H_{22}N_2O_3$
- Bis(4-propoxyphenyl)diazene-1-oxide [23315-55-1]
  4,4'-Dipropoxyazoxybenzene
  Group-member nr.: 62-108

$C_{18}H_{28}O_2Si_3$
- 1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane [797-77-3]
  Group-member nr.: 71-045

$C_{18}H_{28}O_4Si_4$
- 2,2,4,4,6,6-Hexamethyl-8,8-diphenylcyclotetrasiloxane [30026-85-8]
  Group-member nr.: 71-046

$C_{18}H_{30}$
- 3-Ethylhexadecahydropyrene [94262-24-5]
  3-Ethylperhydropyrene
  Group-member nr.: 12-106

$C_{18}H_{30}O_4$
- 1,4-Bis(1,1-diethoxyethyl)benzene [47189-08-2]
  p-Diacetylbenzene tetraethyl ketal
  Ethylacetal *p*-diacetyl benzene
  Group-member nr.: 41-048

$C_{18}H_{32}$
- 1-Cyclohexyloctahydro-1,3,3-trimethyl-1*H*-indene [22236-61-9]
  1-Cyclohexyl-1,3,3-trimethylhydrindan
  Group-member nr.: 12-107
- 1,1':2',1''-Tercyclohexane [2456-43-1]
  o-Tercyclohexane
  Group-member nr.: 12-108
- 1,1':3',1''-Tercyclohexane [1706-50-9]
  m-Tercyclohexane
  Group-member nr.: 12-109
- 1,1':4',1''-Tercyclohexane [1795-19-3]
  p-Tercyclohexane
  Group-member nr.: 12-110

$C_{18}H_{32}O$
- 6,10,14-Trimethyl-3,5-pentadecadien-2-one [1604-32-6]
  Group-member nr.: 43-063

$C_{18}H_{34}$
- 1,1,-Bis(dimethylcyclohexyl)ethane (unspecified isomer) [98803-06-6]
  Group-member nr.: 12-112

- 1,1-Bis(ethylcyclohexyl)ethane (unspecified isomer) [98803-07-7]
  Group-member nr.: 12-111

$C_{18}H_{34}O_2$
- (*Z*)-9-Octadecenoic acid [112-80-1]
  Oleic acid
  Group-member nr.: 44-033

$C_{18}H_{34}O_4$
- Dibutyl decanedioate [109-43-3]
  Dibutyl ester decanedioic acid
  Dibutyl sebacate
  Group-member nr.: 45-105

$C_{18}H_{36}$
- Dodecylcyclohexane [1795-17-1]
  Cyclohexyldodecane
  Group-member nr.: 12-113
- Hexaethylcyclohexane (unspecified isomer) [98803-61-3]
  Group-member nr.: 12-114

$C_{18}H_{36}N_2O_2$
- *N*, *N*'-Dihexylhexanediamide [21150-82-3]
  N, *N*'-Dihexyladipamide
  Group-member nr.: 62-109

$C_{18}H_{36}O$
- 6,10,14-Trimethyl-2-pentadecanone [502-69-2]
  Phytone
  Group-member nr.: 43-064

$C_{18}H_{36}O_2$
- Octadecanoic acid [57-11-4]
  Stearic acid
  Group-member nr.: 44-034

$C_{18}H_{37}Cl$
- 1-Chlorooctadecane [3386-33-2]
  Group-member nr.: 22-049

$C_{18}H_{38}$
- Octadecane [593-45-3]
  Group-member nr.: 11-057

$C_{18}H_{38}O$
- 1-Octadecanol [112-92-5]
  Octadecyl alcohol
  Stearyl alcohol
  Group-member nr.: 42-103

$C_{18}H_{38}S$
- 1,1'-Thiobisnonane [929-98-6]
  10-Thianonadecane
  Dinonyl sulfide
  Group-member nr.: 51-027

$C_{19}H_{16}$
- 1,1',1''-Methylidynetrisbenzene [519-73-3]
  Triphenylmethane
  Tritane
  Group-member nr.: 14-086

$C_{19}H_{22}ClNO$
- 4-Chloro-*N*-[[4-(hexyloxy)phenyl]methylene] benzenamine [5219-48-7]
  p-*n*-Hexyloxybenzylideneamino-*p*'-chlorobenzene
  Group-member nr.: 64-029

$C_{19}H_{22}FNO$
- 4-Fluoro-*N*-[[4-(hexyloxy)]methylene] benzenamine [56544-26-4]
  p-*n*-Hexyloxybenzylideneamino-*p*'-fluorobenzene
  Group-member nr.: 64-030

$C_{19}H_{23}NO$
- 4-Butyl-*N*-[(4-ethoxyphenyl)methylene] benzenamine [29743-08-6]
  p-Butyl-*N*-(*p*-ethoxybenzylidene)aniline
  Group-member nr.: 62-110
- *N*-[[4-(Hexyloxy)phenyl]methylene] benzenamine [5219-49-8]
  p-*n*-Hexyloxybenzylideneaniline
  Group-member nr.: 62-111

$C_{19}H_{36}$
- Bis(2,4,6-trimethylcyclohexyl)methane [94380-80-0]
  Group-member nr.: 12-115
- 4-Heptyl-1,1'-bicyclohexyl [96667-88-8]
  4-Heptylcyclohexylcyclohexane
  Group-member nr.: 12-116
- 1,1'-Heptylidenebiscyclohexane [2090-15-5]
  1,1-Dicyclohexylheptane
  Group-member nr.: 12-117

$C_{19}H_{38}O_2$
- Nonadecanoic acid [646-30-0]
  Nonadecylic acid
  Group-member nr.: 44-035

$C_{19}H_{40}$
- Nonadecane [629-92-5]
  Group-member nr.: 11-058
- 2,6,10,14-Tetramethylpentadecane [1921-70-6]
  Pristane
  Group-member nr.: 11-059

$C_{20}H_{12}$
- Perylene [198-55-0]
  Group-member nr.: 14-087

$C_{20}H_{14}$
- 9,10-Dihydro-9,10[1',2']-benzenoanthracene [477-75-8]
  Triptycene
  Group-member nr.: 14-088

$C_{20}H_{22}N_2O$
- 4-[[[4-(Hexyloxy)phenyl]methylene]amino] - benzonitrile [35280-78-5]
  p-*n*-Hexyloxybenzylideneamino-*p*'-benzonitrile
  Group-member nr.: 62-112

$C_{20}H_{24}N_2O_3$
- (*E*)-4-[(4-Methoxyphenyl)azo]phenyl ester heptanoic acid [97402-83-0]
  Group-member nr.: 62-113

$C_{20}H_{25}NO$
- *N*-[[4-(Hexyloxy)phenyl]methylene]-4-methyl-benzenamine [25959-51-7]
  p-*n*-Hexyloxybenzylidene-*p*'-toluidine
  Group-member nr.: 62-114

$C_{20}H_{26}N_2O_3$
- Bis(4-butoxyphenyl)diazene-1-oxide [17051-01-3]
  4,4'-Dibutoxyazoxybenzene
  Group-member nr.: 62-115

$C_{20}H_{30}O_3Si_3$
- 2,2,4,4-Tetraethyl-6,6-diphenylcyclotrisiloxane [108543-32-4]
  Group-member nr.: 71-047

$C_{20}H_{34}$
- Diethylhexadecahydropyrene [26446-93-5]
  Diethylperhydropyrene
  Group-member nr.: 12-118

$C_{20}H_{34}O_5Si_5$
- Octamethyldiphenylcyclopentasiloxane (unspecified isomer) [51134-26-0]
  Group-member nr.: 71-048

$C_{20}H_{38}HgO_4$
- Mercury(2+) salt decanoic acid [27394-49-6]
  Mercury(II) decanoate;
  Mercury(II) caprate
  Group-member nr.: 74-008

$C_{20}H_{38}O$
- 3,7,11,15-Tetramethyl-1-hexadecyn-3-ol [29171-23-1]
  Group-member nr.: 42-104

$C_{20}H_{38}PbO_4$
- Lead(2+) salt decanoic acid [15773-52-1]
  Lead(II) decanoate;
  Lead(II) caprate
  Group-member nr.: 74-009

$C_{20}H_{40}O$
- 3,7,11,15-Tetramethyl-1-hexadecen-3-ol [505-32-8]
  Isophytol
  Group-member nr.: 42-105

$C_{20}H_{40}O_2$
- Eicosanoic acid [506-30-9]
  Icosanic acid;
  Arachidic acid
  Group-member nr.: 44-036

$C_{20}H_{42}$
- Eicosane [112-95-8]
  Icosane
  Group-member nr.: 11-060

$C_{20}H_{42}S$
- 1,1'-Thiobisdecane [693-83-4]
  11-Thiaheneicosane;
  11-Thiahenicosane;
  Didecyl sulfide
  Group-member nr.: 51-028

$C_{20}H_{44}Sn$
- Tetrapentylstannane [3765-65-9]
  Tetrapentyltin
  Group-member nr.: 73-032

$C_{21}H_{14}N_2O_4$
- 1,1'-(Methylenedi-4,1-phenylene)bis-1*H*-pyrrole-2,5-dione [13676-54-5]
  Bis-(4-maleic acidimidphenyl)methane
  Group-member nr.: 62-116

$C_{21}H_{16}$
- 1-(2-Naphthalenylmethyl)naphthalene [611-48-3]
  1,2'-Dinaphthylmethane
  Group-member nr.: 14-089

$C_{21}H_{21}O_4P$
- Tris(methylphenyl) ester phosphoric acid [1330-78-5]
  Tricresyl phosphate;
  Tritolyl phosphate (unspecified isomer)
  Group-member nr.: 72-014

$C_{21}H_{24}O_3Si_3$
- (2α,4α,6α)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane [3424-57-5]
  cis-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
  Group-member nr.: 71-049
- (2α,4α,6β)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane [6138-53-0]
  trans-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
  Group-member nr.: 71-050

$C_{21}H_{24}O_4$
- 2,2'-[(1-Methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane [1675-54-3]
  Group-member nr.: 47-045

$C_{21}H_{38}$
- 9-(2-Ethylhexyl)dodecahydrofluorene [95135-48-1]
  9-(2-Ethylhexyl)perhydrofluorene
  Group-member nr.: 12-119

- 1,1',1''-(1-Propanyl-2-ylidene)triscyclohexane [55682-89-8]
  1,1,3-Tricyclohexylpropane
  Group-member nr.: 12-120

$C_{21}H_{38}O_6$
- 1,2,3-Propanetriyl ester hexanoic acid [621-70-5]
  1,2,3-Propanetriyl trihexanoate
  Trihexanoin
  Tricaproin
  Group-member nr.: 45-106

$C_{21}H_{40}$
- 4-Nonyl-1,1'-bicyclohexyl [95135-87-8]
  4-Nonylcyclohexylcyclohexane
  Group-member nr.: 12-121

$C_{21}H_{42}O_4$
- 2,3-Dihydroxypropyl ester octadecanoic acid [123-94-4]
  1-Monostearin
  Group-member nr.: 47-046

$C_{21}H_{44}$
- Heneicosane [629-94-7]
  Henicosane
  Group-member nr.: 11-061

$C_{22}H_{14}$
- Pentacene [135-48-8]
  2,3,6,7-Dibenzoanthracene
  Group-member nr.: 14-090

$C_{22}H_{24}O_6$
- *trans*-Bis(4-methoxyphenyl) ester 1,4-cyclohexanedicarboxylic acid [26379-55-5]
  Di(*p*-methoxyphenyl)-*trans*-cyclohexane-1,4-dicarboxylate
  Group-member nr.: 47-047

$C_{22}H_{29}NO$
- 4-Butyl-*N*-[[4-(pentyloxy)phenyl]methylene]-benzenamine [29743-10-0]
  N-*p*-*n*-Pentyloxybenzylidene-*p*'-*n*-butylaniline
  Group-member nr.: 62-117

$C_{22}H_{30}N_2O_3$
- Bis(4-pentyloxyphenyl)diazene-1-oxide [19482-05-4]
  4,4'-Bis(pentyloxy)azoxybenzene
  Group-member nr.: 62-118

$C_{22}H_{42}O_4$
- Bis(2-ethylhexyl) hexanedioate [103-23-1]
  Bis(2-ethylhexyl) adipate
  Bis(2-ethylhexyl) ester hexanedioic acid
  Group-member nr.: 45-107
- Dihexyl decanedioate [2449-10-7]
  Dihexyl ester decanedioic acid
  Dihexyl sebacate
  Group-member nr.: 45-108

$C_{22}H_{44}N_2O_2$
- *N*, *N*'-Dihexyldecanediamine [31827-03-9]
  N, *N*'-Dihexylsebacamide
  Group-member nr.: 62-119

$C_{22}H_{44}O_2$
- Butyl octadecanoate [123-95-5]
  Butyl ester octadecanoic acid
  Butyl stearate
  Group-member nr.: 45-109

$C_{22}H_{45}Br$
- 1-Bromodocosane [6938-66-5]
  n-Docosyl bromide
  Group-member nr.: 23-039

$C_{22}H_{46}$
- Docosane [629-97-0]
  Group-member nr.: 11-062

$C_{23}H_{31}NO$
- 4-Butyl-*N*-[[4-(hexyloxy)phenyl]methylene]-benzenamine [29743-11-1]
  N-*p*-*n*-Hexyloxybenzylidene-*p*'-*n*-butylaniline
  Group-member nr.: 62-120

$C_{23}H_{44}O_5$
- 3-(Acetyloxy)-2-hydroxypropyl ester octadecanoic acid [820-17-7]
  3-Aceto-1-stearin
  Group-member nr.: 47-048

$C_{23}H_{48}$
- Tricosane [638-67-5]
  Group-member nr.: 11-063

$C_{24}H_{18}$
- 5'-Phenyl-1,1':3',1''-terphenyl [612-71-5]
  1,3,5-Triphenylbenzene
  Group-member nr.: 14-091
- 1,1':3',1'':3'',1'''-Quaterphenyl [1166-18-3]
  m-Quaterphenyl
  Group-member nr.: 14-092

$C_{24}H_{32}O_3$
- 4-(Heptyloxy)phenyl ester 4-butylbenzoic acid [38454-35-2]
  p-(Heptyloxy)phenyl *p*-butylbenzoate
  Group-member nr.: 47-049

$C_{24}H_{34}$
- 1,1-Diphenyldodecane [1603-53-8]
  Group-member nr.: 14-093

$C_{24}H_{34}N_2O_3$
- Bis(4-hexyloxyphenyl)diazene-1-oxide [2587-42-0]
  4,4'-Bis(hexyloxy)azoxybenzene
  Group-member nr.: 62-121

$C_{24}H_{38}O_4$
- Bis(2-ethylhexyl)-1,2-benzenedicarboxylate [117-81-7]
  Bis(2-ethylhexyl) ester phthalic acid
  Group-member nr.: 45-110

$C_{24}H_{40}$
- (1-Cyclohexyldodecyl)benzene [62155-50-4]
  1-Cyclohexyl-1-phenyldodecane
  Group-member nr.: 14-094

$C_{24}H_{46}CdO_4$
- Cadmium salt dodecanoic acid [2605-44-9]
  Cadmium dodecanoate
  Cadmium laurate
  Group-member nr.: 74-010

$C_{24}H_{46}HgO_4$
- Mercury(2+) salt dodecanoic acid [23186-25-6]
  Mercury(II) dodecanoate
  Mercury(II) laurate
  Group-member nr.: 74-011

$C_{24}H_{46}O_4Pb$
- Lead(2+) salt dodecanoic acid [15773-55-4]
  Lead(II) dodecanoate
  Lead(II) laurate
  Group-member nr.: 74-012

$C_{24}H_{50}$
- Tetracosane [646-31-1]
  Group-member nr.: 11-064

$C_{24}H_{52}ClNO_4$
- *N*, *N*, *N*-Trihexyl-1-hexanaminium perchlorate [4656-81-9]
  Tetrahexylammonium perchlorate
  Group-member nr.: 74-013

$C_{24}H_{52}O_4Si$
- Tetrakis(2-ethylbutyl) ester silicic acid [78-13-7]
  Tetrakis(2-ethylbutyl) orthosilicate
  Tetrakis(2-ethylbutoxy)silane
  Group-member nr.: 71-051

$C_{25}H_{46}$
- 4'-Heptyl-1,1':3',1''-tercyclohexane [unknown]
  4-Heptyl-*m*-tercyclohexyl
  Group-member nr.: 12-122

$C_{25}H_{46}O_6$
- 2,3-Bis(acetyloxy)propyl ester octadecanoic acid [33599-07-4]
  1,2-Diacetostearin
  Group-member nr.: 45-111

$C_{25}H_{48}O_4$
- Bis(2-ethylhexyl) nonanedioate [103-24-2]
  Bis(2-ethylhexyl) azelate
  Bis(2-ethylhexyl) ester nonanedioic acid
  Group-member nr.: 45-112

$C_{25}H_{52}$
- Pentacosane [629-99-2]
  Group-member nr.: 11-065

$C_{26}H_{18}$
- 9,10-Diphenylanthracene [1499-10-1]
  Group-member nr.: 14-095

$C_{26}H_{26}OSi_2$
- 1,3-Dimethyl-1,1,3,3-tetraphenyldisiloxane [807-28-3]
  Group-member nr.: 71-052

$C_{26}H_{36}O_3Si_3$
- 2,2-Dimethyl-4,4,6,6-tetraphenylcyclotrisiloxane [1438-86-4]
  Group-member nr.: 71-053

$C_{26}H_{38}N_2O_3$
- Bis(4-heptyloxyphenyl)diazene-1-oxide [2635-26-9]
  4,4'-Bis(heptyloxy)azoxybenzene
  Group-member nr.: 62-122

$C_{26}H_{50}O_4$
- Dioctyl decanedioate [2432-87-3]
  Dioctyl ester decanedioic acid
  Dioctyl sebacate
  Group-member nr.: 45-113

$C_{26}H_{54}$
- Hexacosane [630-01-3]
  Group-member nr.: 11-066

$C_{27}H_{48}$
- 11-Phenylheneicosane [6703-80-6]
  (1-Decylundecyl)benzene
  11-Phenylhenicosane
  Group-member nr.: 14-096

$C_{27}H_{50}$
- 4'-Nonyl-1,1':3',1''-tercyclohexane [unknown]
  4-Nonyl-*m*-tercyclohexyl
  Group-member nr.: 12-123

$C_{27}H_{50}O_6$
- 1,2,3-Propanetriyl ester octanoic acid [538-23-8]
  1,2,3-Propanetriyl trioctanoate
  Trioctanoin
  Group-member nr.: 45-114

$C_{27}H_{54}$
- (1-Decylundecyl)cyclohexane [6703-99-7]
  11-Cyclohexylheneicosane
  11-Cyclohexylhenicosane
  Group-member nr.: 12-124

$C_{27}H_{56}$
- Heptacosane [593-49-7]
  Group-member nr.: 11-067

$C_{28}H_{28}P$
- 1,4-Butanediylbis(diphenylphosphine) [7688-25-7]
  1,4-Bis(diphenylphosphino)butane
  Tetramethylenebis(diphenylphosphine)
  Group-member nr.: 72-015

$C_{28}H_{32}O_4Si_4$
- 2,2,4,4-Tetramethyl-6,6,8,8-tetraphenylcyclotetrasiloxane [1693-47-6]
  Group-member nr.: 71-054
- 2,4,6,8-Tetramethyl-2,4,6,8-tetraphenylcyclotetrasiloxane [77-63-4]
  Group-member nr.: 71-055

$C_{28}H_{42}N_2O_3$
- Bis(4-octyloxyphenyl)diazene-1-oxide [25729-12-8]
  4,4'-Bis(octyloxy)azoxybenzene
  Group-member nr.: 62-123

$C_{28}H_{54}CdO_4$
- Cadmium salt tetradecanoic acid [10196-67-5]
  Cadmium tetradecanoate
  Cadmium myristate
  Group-member nr.: 74-014

$C_{28}H_{54}HgO_4$
- Mercury(2+) salt tetradecanoic acid [36215-49-3]
  Mercury(II) tetradecanoate
  Mercury(II) myristate
  Group-member nr.: 74-015

$C_{28}H_{54}O_4Pb$
- Lead(2+) salt tetradecanoic acid [32112-52-0]
  Lead(II) tetradecanoate
  Lead(II) myristate
  Group-member nr.: 74-016

$C_{28}H_{58}$
- Octacosane [630-02-4]
  Group-member nr.: 11-068

$C_{29}H_{42}O_4$
- 4-(Hexyloxy)phenyl ester 4-(decyloxy)benzoic acid [68162-09-4]
  4-Hexyloxyphenyl-4'-*n*-decyloxybenzoate
  Group-member nr.: 47-050

$C_{30}H_{46}N_2O_3$
- Bis(4-nonyloxyphenyl)diazene-1-oxide [25729-13-9]
  4,4'-Bis(nonyloxy)azoxybenzene
  Group-member nr.: 62-124

$C_{30}H_{58}O_4$
- Didecyl decanedioate [2432-89-5]
  Didecyl ester decanedioic acid
  Didecyl sebacate
  Group-member nr.: 45-115

$C_{30}H_{61}Br$
- 1-Bromotriacontane [4209-22-7]
  n-Triacontyl bromide
  Group-member nr.: 23-040

$C_{30}H_{62}$
- 2,6,10,15,19,23-Hexamethyltetracosane [111-01-3]
  Squalane
  Group-member nr.: 11-069
- Triacontane [638-68-6]
  Group-member nr.: 11-070

$C_{31}H_{52}O_3$
- 3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol acetate [7695-91-2]
  α-Tocopherol acetate
  Group-member nr.: 47-051

$C_{31}H_{64}$
- 11-Decylheneicosane [55320-06-4]
  11-Decylhenicosane
  Group-member nr.: 11-071
- Hentriacontane [630-04-6]
  Unatriacontane
  Group-member nr.: 11-072

$C_{32}H_{50}N_2O_3$
- Bis(4-decyloxyphenyl)diazene-1-oxide [2312-12-1]
  4,4'-Bis(decyloxy)azoxybenzene
  Group-member nr.: 62-125

$C_{32}H_{62}CdO_4$
- Cadmium salt hexadecanoic acid [6427-86-7]
  Cadmium hexadecanoate
  Cadmium palmitate
  Group-member nr.: 74-017

$C_{32}H_{62}HgO_4$
- Mercury(2+) salt hexadecanoic acid [16888-60-1]
  Mercury(II) hexadecanoate
  Mercury(II) palmitate
  Group-member nr.: 74-018

$C_{32}H_{62}O_4Pb$
- Lead(2+) salt hexadecanoic acid [15773-56-5]
  Lead(II) hexadecanoate
  Lead(II) palmitate
  Group-member nr.: 74-019

$C_{32}H_{66}$
- Dotriacontane [544-85-4]
  Group-member nr.: 11-073

$C_{33}H_{62}O_6$
- 1,2,3-Propanetriyl ester decanoic acid [621-71-6]
  1,2,3-Propanetriyl tridecanoate
  Tridecanoin
  Group-member nr.: 45-116

$C_{33}H_{68}$
- Tritriacontane [630-05-7]
  Group-member nr.: 11-074

$C_{34}H_{54}N_2O_3$
- Bis[4-(undecyloxy)phenyl]diazene-1-oxide [2312-13-2]
  4,4'-Bis(undecyloxy)azoxybenzene
  Group-member nr.: 62-126

$C_{34}H_{66}O_4$
- Didodecyl decanedioate [2432-88-4]
  Didodecyl ester decanedioic acid
  Didodecyl sebacate
  Group-member nr.: 45-117

$C_{34}H_{70}$
- Tetratriacontane [14167-59-0]
  Group-member nr.: 11-075

$C_{35}H_{72}$
- Pentatriacontane [630-07-9]
  Group-member nr.: 11-076

$C_{36}H_{24}$
- 1,1',1''-(1,3,5-Benzenetriyl)trisnaphthalene [7059-70-3]
  1,3,5-Tri-α-naphthylbenzene
  Group-member nr.: 14-097

$C_{36}H_{58}N_2O_3$
- Bis[4-(dodecyloxy)phenyl]diazene-1-oxide [2312-14-3]
  4,4'-Bis(dodecyloxy)azoxybenzene
  Group-member nr.: 62-127

$C_{36}H_{70}CdO_4$
- Cadmium salt octadecanoic acid [2223-93-0]
  Cadmium octadecanoate
  Cadmium stearate
  Group-member nr.: 74-020

$C_{36}H_{70}HgO_4$
- Mercury(2+) salt octadecanoic acid [645-99-8]
  Mercury(II) octadecanoate
  Mercury(II) stearate
  Group-member nr.: 74-021

$C_{36}H_{70}O_4Pb$
- Lead(2+) salt octadecanoic acid [1072-35-1]
  Lead(II) octadecanoate
  Lead(II) stearate
  Group-member nr.: 74-022

$C_{36}H_{74}$
- Hexatriacontane [630-06-8]
  Group-member nr.: 11-077

$C_{37}H_{54}Si$
- Tribenzylhexadecylsilane [4033-52-7]
  Group-member nr.: 71-056

$C_{38}H_{70}O_8$
- 1,6-Hexanediyldihexyl ester decanedioic acid [55205-81-7]
  Dihexyl hexamethylenesebacate
  Group-member nr.: 45-118

$C_{38}H_{74}O_4$
- Ditetradecyl decanedioate [26719-47-1]
  Ditetradecyl ester decanedioic acid
  Ditetradecyl sebacate
  Group-member nr.: 45-119

$C_{39}H_{74}O_6$
- 1,2,3-Propanetriyl ester dodecanoic acid [538-24-9]
  1,2,3-Propanetriyl tridodecanoate
  Trilaurin
  Group-member nr.: 45-120

$C_{40}H_{82}$
- Tetracontane [4181-95-7]
  Group-member nr.: 11-078

$C_{41}H_{72}O_2$
- Cholest-5-en-3-ol (3β) tetradecanoate [1989-52-2]
  Cholesterol myristate
  Group-member nr.: 45-121

$C_{42}H_{66}O_{12}$
- 1,2,3,4,5,6-Benzenehexayl ester hexanoic acid [65201-69-6]
  Benzene hexa-*n*-hexanoate
  Group-member nr.: 45-122

$C_{42}H_{82}O_4$
- Dihexadecyl decanedioate [26719-48-2]
  Dihexadecyl ester decanedioic acid
  Dihexadecyl sebacate
  Group-member nr.: 45-123

$C_{42}H_{86}$
- Dotetracontane [7098-20-6]
  Group-member nr.: 11-079

$C_{43}H_{88}$
- Tritetracontane [7098-21-7]
  Group-member nr.: 11-080

$C_{44}H_{90}$
- Tetratetracontane [7098-22-8]
  Group-member nr.: 11-081

$C_{45}H_{86}O_6$
- 1,2,3-Propanetriyl ester tetradecanoic acid [555-45-3]
  1,2,3-Propanetriyl tritetradecanoate
  Trimyristin
  Group-member nr.: 45-124

$C_{46}H_{90}O_4$
- Dioctadecyl decanedioate [3072-03-5]
  Dioctadecyl ester decanedioic acid
  Dioctadecyl sebacate
  Group-member nr.: 45-125

$C_{48}H_{78}O_{12}$
- 1,2,3,4,5,6-Benzenehexayl ester heptanoic acid [65201-70-9]
  Benzene hexa-*n*-heptanoate
  Group-member nr.: 45-126

$C_{48}H_{98}$
- Octatetracontane [7098-26-2]
  Group-member nr.: 11-082

$C_{50}H_{102}$
- Pentacontane [6596-40-3]
  Group-member nr.: 11-083

$C_{51}H_{98}O_6$
- 1,2,3-Propanetriyl ester hexadecanoic acid [555-44-2]
  1,2,3-Propanetriyl trihexadecanoate
  Tripalmitin
  Group-member nr.: 45-127

$C_{54}H_{90}O_{12}$
- 1,2,3,4,5,6-Benzenehexayl ester octanoic acid [65201-71-0]
  Benzene hexa-*n*-octanoate
  Group-member nr.: 45-128

$C_{54}H_{98}O_{12}$
- 10,19,28,37-Tetraoxodihexyl ester 11,18,29,36-tetraoxahexatetracosanedioic acid [55205-82-8]
  Dihexyl bis(hexamethylenesebacate)
  Group-member nr.: 45-129

$C_{57}H_{110}O_6$
- 1,2,3-Propanetriyl ester octadecanoic acid [555-43-1]
  1,2,3-Propanetriyl trioctadecanoate
  Tristearin
  Group-member nr.: 45-130

ClD
- Hydrochlorid acid-*d* [7698-05-7]
  Deuterium chloride
  Group-member nr.: 02-030

$ClFO_3$
- Perchloryl fluoride ($(ClO_3)F$) [7616-94-6]
  Group-member nr.: 02-031

ClF_3
- Chlorine fluoride (ClF_3) [7790-91-2]
  Chlorine trifluoride
  Group-member nr.: 02-032

ClH
- Hydrochlorid acid [7647-01-0]
  Hydrogen chloride
  Group-member nr.: 02-033

$ClHO_4$
- Perchloric acid [7601-90-3]
  Group-member nr.: 02-034

ClI
- Iodine chloride [7790-99-0]
  Iodine monochloride
  Group-member nr.: 02-035

$ClNaO_3$
- Sodium salt chloric acid [7775-09-9]
  Sodium chlorate
  Group-member nr.: 02-036

Cl_2
- Chlorine [7782-50-5]
  Group-member nr.: 01-004

Cl_2OS
- Thionyl chloride [7719-09-7]
  Group-member nr.: 02-037

Cl_2O_2S
- Sulfuryl chloride [7791-25-5]
  Group-member nr.: 02-038

$Cl_2O_5S_2$
- Disulfuryl chloride [7791-27-7]
  Pyrosulfuryl chloride
  Group-member nr.: 02-039

Cl_2S_2
- Sulfur chloride (S_2Cl_2) [10025-67-9]
  Sulfur monochloride
  Group-member nr.: 02-040

Cl_2Sn
- Tin chloride ($SnCl_2$) [7772-99-8]
  Group-member nr.: 02-041

Cl_3HSi
- Trichlorosilane [10025-78-2]
  Group-member nr.: 02-042

Cl_3OP
- Phosphoryl chloride [10025-87-3]
  Group-member nr.: 02-043

Cl_3P
- Phosphorous trichloride [7719-12-2]
  Phosphorus chloride (PCl_3)
  Group-member nr.: 02-044

Cl_4Ge
- Tetrachlorogermane [10038-98-9]
  Germanium tetrachloride
  Group-member nr.: 02-045

Cl_4Si
- Tetrachlorosilane [10026-04-7]
  Silicon chloride
  Group-member nr.: 02-046

Cl_4Sn
- Tetrachlorostannane [7646-78-8]
  Tin(IV) chloride
  Tin tetrachloride
  Group-member nr.: 02-047

Cl_4Te
- Tellurium chloride ($TeCl_4$) [10026-07-0]
  Tellurium tetrachloride
  Group-member nr.: 02-048

Cl_4Ti
- Titanium chloride ($TiCl_4$) [7550-45-0]
  Titanium tetrachloride
  Titanic chloride
  Group-member nr.: 02-049

Cs
- Cesium [7440-46-2]
  Group-member nr.: 01-005

CsF_2H
- Cesium fluoride ($Cs(HF_2)$) [12280-52-3]
  Cesium hydrogen difluoride
  Group-member nr.: 02-050

DH
- Deuterium molecule with hydrogen [13983-20-5]
  Hydrogen deuteride
  Group-member nr.: 02-051

DI
- Hydroiodic acid-*d* [14104-45-1]
  Deuterium iodide
  Group-member nr.: 02-052

D_2
- Deuterium (D_2) [7782-39-0]
  Group-member nr.: 01-006
- *ortho*-Deuterium (D_2) [7782-39-0]
  Group-member nr.: 01-007

D_2O
- Water-d_2 [7789-20-0]
  Heavy water
  Deuterium oxide
  Group-member nr.: 02-053

D_2O_2
- Hydrogen-d_2 peroxide [6909-54-2]
  Deuterium peroxide
  Group-member nr.: 02-054

D_2S
- Hydrogen sulfide-d_2 [13536-94-2]
  Deuterium sulfide
  Group-member nr.: 02-055

D_2Se
- Hydrogen selenide-d_2 [13536-95-3]
  Deuterium selenide
  Group-member nr.: 02-056

D_3N
- Ammonia-d_3 [13550-49-7]
  Deuterium ammonia
  Trideuterated ammonia
  Group-member nr.: 02-057

FH
- Hydrofluoric acid [7664-39-3]
  Hydrogen fluoride
  Group-member nr.: 02-058

F_2
- Fluorine [7782-41-4]
  Group-member nr.: 01-008

F_2HRb
- Rubidium fluoride ($Rb(HF_2)$) [12280-64-7]
  Rubidium hydrogen difluoride
  Group-member nr.: 02-059

F_2H_5N
- Ammonium fluoride ($(NH_4)(HF_2)$) [1341-49-7]
  Ammonium hydrogen difluoride
  Group-member nr.: 02-060

F_2O
- Oxygen fluoride [7783-41-7]
  Group-member nr.: 02-061

F_2OS
- Thionyl fluoride [7783-42-8]
  Group-member nr.: 02-062

F_2O_2S
- Sulfuryl fluoride [2699-79-8]
  Group-member nr.: 02-063

F_3N
- Nitrogen fluoride (NF_3) [7783-54-2]
  Nitrogen trifluoride
  Group-member nr.: 02-064

F_3OP
- Phosphoryl fluoride [13478-20-1]
  Group-member nr.: 02-065

F_3P
- Phosphorous trifluoride [7783-55-3]
  Phosphorus trifluoride
  Phosphorous fluoride (PF_3)
  Group-member nr.: 02-066

F_5I
- Iodine fluoride (IF_5) [7783-66-6]
  Iodine pentafluoride
  Group-member nr.: 02-067

F_5Nb
- Niobium fluoride (NbF_5) [7783-68-8]
  Niobium pentafluoride
  Group-member nr.: 02-068

F_6Mo
- Molybdenum fluoride (MoF_6) [7783-77-9]
  Molybdenum hexafluoride
  Group-member nr.: 02-069

F_6S
- Sulfur fluoride (SF_6) [2551-62-4]
  Sulfur hexafluoride
  Group-member nr.: 02-070

F_6U
- Uranium(VI) fluoride [7783-81-5]
  Uranium hexafluoride
  Group-member nr.: 02-071

Ga
- Gallium [7440-55-3]
  Group-member nr.: 01-009

GeH_4
- Germane [7782-65-2]
  Group-member nr.: 02-072

HI
- Hydroiodic acid [10034-85-2]
  Hydrogen iodide
  Group-member nr.: 02-073

HNO_3
- Nitric acid [7697-37-2]
  Group-member nr.: 02-074

H_2
- Hydrogen [1333-74-0]
  Group-member nr.: 01-010
- *para*-Hydrogen [1333-74-0]
  Group-member nr.: 01-011

H_2O
- Water [7732-18-5]
  Group-member nr.: 02-075

H_2O_2
- Hydrogen peroxide [7722-84-1]
  Group-member nr.: 02-076

H_2O_4S
- Sulfuric acid [7664-93-9]
  Group-member nr.: 02-077

$H_2O_7S_2$
- Disulfuric acid [7783-05-3]
  Pyrosulfuric acid
  Group-member nr.: 02-078

H_2S
- Hydrogen sulfide [7783-06-4]
  Group-member nr.: 02-079

H_2S_2
- Hydrogen sulfide (H_2S_2) [13465-07-1]
  Dihydrogen disulfide
  Group-member nr.: 02-080

H_2S_3
- Hydrogen sulfide (H_2S_3) [13845-23-3]
  Dihydrogen trisulfide
  Group-member nr.: 02-081

H_2S_4
- Hydrogen sulfide (H_2S_4) [13845-25-5]
  Dihydrogen tetrasulfide
  Group-member nr.: 02-082

H_2S_5
- Hydrogen sulfide (H_2S_5) [13845-24-4]
  Dihydrogen pentasulfide
  Group-member nr.: 02-083

H_2S_6
- Hydrogen sulfide (H_2S_6) [13845-51-7]
  Dihydrogen hexasulfide
  Group-member nr.: 02-084

H_2Se
- Hydrogen selenide [7783-07-5]
  Group-member nr.: 02-085

H_3N
- Ammonia [7664-41-7]
  Group-member nr.: 02-086

H_3O_4P
- Phosphoric acid [7664-38-2]
  Group-member nr.: 02-087

H_3P
- Phosphine [7803-51-2]
  Group-member nr.: 02-088

H_4N_2
- Hydrazine [302-01-2]
  Group-member nr.: 02-089

H_4Si
- Silane [7803-62-5]
  Group-member nr.: 02-090

H_5NO
- Ammonium hydroxide [1336-21-6]
  Group-member nr.: 02-091

$H_5N_3O_3$
- Hydrazine mononitrate [13464-97-6]
  Hydrazine nitrate
  Group-member nr.: 02-092

H_8N_2O
- Ammonium oxide [12161-77-2]
  Group-member nr.: 02-093

He
- Helium [7440-59-7]
  Group-member nr.: 01-012
- Helium (isotope of mass 3) [14762-55-1]
  Group-member nr.: 01-013

Hg
- Mercury [7439-97-6]
  Group-member nr.: 01-014

HgI_2
- Mercury iodide (HgI_2) [7774-29-0]
  Group-member nr.: 02-094

I_2
- Iodine [7553-56-2]
  Group-member nr.: 01-015

I_4Sn
- Tetraiodostannane [7790-47-8]
  Tin iodide
  Stannic iodide
  Group-member nr.: 02-095

In
- Indium [7440-74-6]
  Group-member nr.: 01-016

K
- Potassium [7440-09-7]
  Kalium
  Group-member nr.: 01-017

Kr
- Krypton [7439-90-9]
  Group-member nr.: 01-018

Li
- Lithium [7439-93-2]
  Group-member nr.: 01-019

$LiNO_3$
- Lithium salt nitric acid [7790-69-4]
  Lithium nitrate
  Group-member nr.: 02-096

NO
- Nitrogen oxide (NO) [10102-43-9]
  Nitrogen monoxide
  Nitric oxide
  Group-member nr.: 02-097

NO_2
- Nitrogen oxide (NO_2) [10102-44-0]
  Nitrogen dioxide
  Group-member nr.: 02-098

N_2
- Nitrogen [7727-37-9]
  Group-member nr.: 01-020

N_2O
- Nitrogen oxide (N_2O) [10024-97-2]
  Dinitrogen monoxide
  Nitrous oxide
  Group-member nr.: 02-099

N_2O_4
- Nitrogen oxide (N_2O_4) [10544-72-6]
  Dinitrogen tetroxide
  Nitrogen peroxide
  Nitrogen tetroxide
  Group-member nr.: 02-100

Na
- Sodium [7440-23-5]
  Natrium
  Group-member nr.: 01-021

Ne
- Neon [7440-01-9]
  Group-member nr.: 01-022

O_2
- Oxygen [7782-44-7]
  Group-member nr.: 01-023

O_2S
- Sulfur dioxide [7446-09-5]
  Group-member nr.: 02-101

O_3
- Ozone [10028-15-6]
  Group-member nr.: 01-024

O_3S
- Sulfur trioxide [7446-11-9]
  Group-member nr.: 02-102

O_6P_4
- Phosphorus oxide (P_4O_6) [12440-00-5]
  Group-member nr.: 02-103

P_4
- Phosphorus mol.(P_4) [12185-10-3]
  Group-member nr.: 01-025

Rb
- Rubidium [7440-17-7]
  Group-member nr.: 01-026

S
- Sulfur [7704-34-9]
  Group-member nr.: 01-027

Se
- Selenium [7782-49-2]
  Group-member nr.: 01-028

Sn
- Tin [7440-31-5]
  Stannane
  Group-member nr.: 01-029

Xe
- Xenon [7440-63-3]
  Group-member nr.: 01-030

Name Index of Compounds

1-[2-[(2-Aminoethyl)amino]ethyl]piperazine	*see* *N*-[2-(1-Piperazinyl)ethyl]-1,2-ethanediamine
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1-(2-Aminoethyl)piperazine	*see* 1-Piperazineethanamine
N-(2-Aminoethyl)-1,4-piperazinediethanamine	33-041
6-Aminohexanoic lactam	*see* Hexahydro-2*H*-azepin-2-one
2-Amino-2-(hydroxymethyl)-1,3-propanediol	62-032
Aminomethane	*see* Methanamine
2-Amino-2-methyl-1,3-propanediol	62-031
2-Amino-2-methyl-1-propanol	62-028
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4-Aminophenyl sulfone	*see* 4,4'-Sulfonylbisbenzenamine
3-Aminopropyltriethoxysilane	*see* 3-(Triethoxysilyl)-1-propanamine
Aminotoluene	*see* Benzenemethanamine
Ammonia	02-086
Ammonia-d_3	02-057
Ammonium fluoride ($(NH_4)(HF_2)$)	02-060
Ammonium hydrogen difluoride	*see* Ammonium fluoride ($(NH_4)(HF_2)$)
Ammonium hydroxide	02-091
Ammonium oxide	02-093
Amyl acetate	*see* Pentyl acetate
n-Amyl alcohol	*see* 1-Pentanol
sec-Amyl alcohol	*see* 2-Pentanol
tert-Amyl alcohol	*see* 2-Methyl-2-butanol
Amyl aldehyde	*see* Pentanal
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n-Amyl bromide	*see* 1-Bromopentane
Amyl butyrate	*see* Pentyl butanoate
Amyl cyanide	*see* Hexanenitrile
β-Amylene	*see* 2-Pentene
cis-β-Amylene	*see* (*Z*)-2-Pentene
trans-β-Amylene	*see* (*E*)-2-Pentene
tert-Amyl ethyl ether	*see* 2-Ethoxy-2-methylbutane
tert-Amyl mercaptan	*see* 2-Methyl-2-butanethiol
tert-Amyl methyl ether	*see* 2-Methoxy-2-methylbutane
Amyl propionate	*see* Pentyl propanoate
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Aniline	*see* Benzenamine
Anisaldazine	*see* [(4-Methoxyphenyl)methylene]hydrazone-4-methoxybenzaldehyde
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1-Butyldecalin	*see* 1-Butyldecahydronaphthalene
α-*sec*-Butyldecalin	*see* Decahydro-1-(1-methylpropyl)naphthalene
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2-Butyl mercaptan	*see* 2-Butanethiol

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Cadmium hexadecanoate	*see* Cadmium salt hexadecanoic acid
Cadmium laurate	*see* Cadmium salt dodecanoic acid
Cadmium myristate	*see* Cadmium salt tetradecanoic acid
Cadmium octadecanoate	*see* Cadmium salt octadecanoic acid
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1-Cyanobicyclo[3.1.0]hexane	*see* Bicyclo[3.1.0]hexane-1-carbonitrile
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Cyanocyclohexane	*see* Cyclohexanecarbonitrile
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11-Cyclohexylhenicosane	*see* (1-Decylundecyl)cyclohexane
1-Cyclohexyl-1-(isopropylcyclohexyl)ethane (unspecified isomer)	*see* 1-Cyclohexyl-1-(1-methylethyl)cyclohexylethane
Cyclohexyl(isopropylcyclohexyl)methane (unspecified isomer)	*see* Cyclohexyl[(1-methylethyl)cyclohexyl]methane
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p-Diacetylbenzene tetraethyl ketal	*see* 1,4-Bis(1,1-diethoxyethyl)benzene
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Diallyl succinate	*see* Di-2-propenyl butanedioate
Diamantane	*see* Decahydro-3,5,1,7-[1,2,3,4]butanetetraylnaphthalene
4,4'-Diaminodiphenyl ether	*see* 4,4'-Oxybisbenzenamine
1,2-Diaminoethane	*see* 1,2-Ethanediamine
1,2-Diamino-2-methylpropane	*see* 2-Methyl-1,2-propanediamine
1,2-Diaminopropane (racemic)	*see* (*R,S*)-1,2-Propanediamine
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N, *N*'-Dihexylhexanediamide	62-109
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Dihexyl sebacate	*see* Dihexyl decanedioate
Dihexyl sulfide	*see* 1,1'-Thiobishexane
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2,3-Dihydroindene	14-026
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p-Dihydroxybenzene	*see* 1,4-Benzenediol
1,2-Dihydroxybenzene	*see* 1,2-Benzenediol
1,3-Dihydroxybenzene	*see* 1,3-Benzenediol
1,4-Dihydroxybenzene	*see* 1,4-Benzenediol
2,2'-Dihydroxydiethyl ether	*see* 2,2'-Oxybisethanol
1,8-Dihydroxy-3,6-dioxaoctane	*see* 2,2'-[1,2-Ethanediylbis(oxy)]bisethanol
4,4'-Dihydroxydiphenyl-2,2-propane	*see* 4,4'-(1-Methylethylidene)bisphenol
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Diisoamyl succinate	*see* Bis(3-methylbutyl) butanedioate
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Diisobutyl ketone	*see* 2,6-Dimethyl-4-heptanone
Diisobutyl oxalate	*see* Bis(2-methylpropyl) ethanedioate
Diisobutyl succinate	*see* Bis(2-methylpropyl) butanedioate
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Diisopropyl ketone	*see* 2,4-Dimethyl-3-pentanone
Diisopropyl sulfide	*see* 2,2'-Thiobispropane
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4,4'-Dimethoxyazoxybenzene	*see* Bis(4-methoxyphenyl)diazene-1-oxide
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Dimethyl carbonate	45-004
1,1-Dimethylcyclohexane	12-029
cis-1,2-Dimethylcyclohexane	12-030
trans-1,2-Dimethylcyclohexane	12-031
cis-1,3-Dimethylcyclohexane	12-032
trans-1,3-Dimethylcyclohexane	12-033
cis-1,4-Dimethylcyclohexane	12-034
trans-1,4-Dimethylcyclohexane	12-035
1,1-Dimethylcyclopentane	12-014
cis-1,2-Dimethylcyclopentane	12-015
trans-1,2-Dimethylcyclopentane	12-016
trans-1,3-Dimethylcyclopentane	12-017
Dimethyldecalin (unspecified isomer)	*see* Decahydrodimethylnaphthalene
3,6-Dimethyl-1,4-dioxane-2,5-dione	47-018

(4-Ethoxyphenyl)(4-methoxyphenyl)diazene-*N*-oxide	62-100
1-Ethoxypropane	41-008
1-Ethoxy-2-propoxyethane	41-029
Ethylacetal *p*-diacetyl benzene	*see* 1,4-Bis(1,1-diethoxyethyl)benzene
N-Ethylacetamide	62-025
Ethyl acetate	45-007
Ethylacetic acid	*see* Butanoic acid
Ethyl acetoacetate	*see* Ethyl ester 3-oxobutanoic acid
4'-Ethylacetophenone	*see* 1-(4-Ethylphenyl)ethanone
Ethylacetylene	*see* 1-Butyne
Ethyl alcohol	*see* Ethanol
Ethylamine	*see* Ethanamine
Ethylammonium nitrate	*see* Nitrate ethylamine
Ethyl-*p,p*-azoxybenzoate	*see* Diethyl ester 4,4'-azoxybisbenzoic acid
Ethylbenzene	14-021
Ethyl benzenepropanoate	45-088
Ethyl benzoate	45-064
2-Ethyl-1,1'-bicyclohexyl	12-090
Ethyl bromide	*see* Bromoethane
Ethyl butanoate	45-029
2-Ethyl-1-butanol	42-040
2-Ethylbutyl alcohol	*see* 2-Ethyl-1-butanol
Ethyl butyrate	*see* Ethyl butanoate
Ethyl caproate	*see* Ethyl hexanoate
Ethyl carbamate	*see* Ethyl ester carbamic acid
Ethyl carbonate	*see* Diethyl carbonate
Ethyl cellosolve	*see* 2-Ethoxyethanol
Ethyl chloride	*see* Chloroethane
Ethyl chloroacetate	61-021
Ethyl 2-chloropropanoate	61-032
Ethyl α-chloropropionate	*see* Ethyl 2-chloropropanoate
Ethyl cinnamate (unspecified stereoisomer)	*see* Ethyl 3-phenyl-2-propenoate
Ethyl cyanide	*see* Propanenitrile
Ethyl cyanoacetate	*see* Ethyl ester cyanoacetic acid
Ethylcyclohexane	12-036
Ethyl cyclohexanecarboxylate	45-067
2-Ethylcyclohexylcyclohexane	*see* 2-Ethyl-1,1'-bicyclohexyl
Ethylcyclopentane	12-018
1-Ethylcyclopentene	14-013
Ethyl cyclopropanecarboxylate	45-022
Ethyldecahydronaphthalene	12-067
1-Ethyldecahydronaphthalene	12-068
2-Ethyldecahydronaphthalene	12-069
Ethyldecalin (unspecified isomer)	*see* Ethyldecahydronaphthalene
α-Ethyldecalin	*see* 1-Ethyldecahydronaphthalene
β-Ethyldecalin	*see* 2-Ethyldecahydronaphthalene
1-Ethyldecalin	*see* 1-Ethyldecahydronaphthalene
2-Ethyldecalin	*see* 2-Ethyldecahydronaphthalene
Ethyl dichloroacetate	61-018
Ethyl 2,3-dichloropropanoate	61-029
Ethyl 2,2-dimethylpropanoate	45-040
S-Ethyl dipropylthiocarbamate	*see S*-Ethyl ester dipropylcarbamothionic acid
Ethyl disulfide	*see* 3,4-Dithiahexane
Ethylene	*see* Ethene
Ethylene carbonate	*see* 1,3-Dioxolan-2-one
Ethylene chlorobromide	*see* 1-Bromo-2-chloroethane
Ethylenediamine	*see* 1,2-Ethanediamine
Ethylene dibromide	*see* 1,2-Dibromoethane
Ethylene dichloride	*see* 1,2-Dichloroethane

Ethylene dicyanide	*see* Butanedinitrile
Ethylene glycol	*see* 1,2-Ethanediol
Ethylene glycol butyl ether methyl ether	*see* 1-Butoxy-2-methoxyethane
Ethylene glycol diacetate	*see* 1,2-Ethanediyl diacetate
Ethylene glycol dibutyl ether	*see* 1,1'-[1,2-Ethanediylbis(oxy)]bisbutane
Ethylene glycol dibutyrate	*see* 1,2-Ethanediyl dibutanoate
Ethylene glycol diethyl ether	*see* 1,2-Diethoxyethane
Ethylene glycol dimethyl ether	*see* 1,2-Dimethoxyethane
Ethylene glycol dipropionate	*see* 1,2-Ethanediyl dipropanoate
Ethylene glycol dipropyl ether	*see* 1,2-Dipropoxyethane
Ethylene glycol ethyl ether methyl ether	*see* 1-Ethoxy-2-methoxyethane
Ethylene glycol ethyl ether propyl ether	*see* 1-Ethoxy-2-propoxyethane
Ethylene glycol methyl ether propyl ether	*see* 1-Methoxy-2-propoxyethane
Ethylene glycol monobutyl ether	*see* 2-Butoxyethanol
Ethylene glycol monoethyl ether	*see* 2-Ethoxyethanol
Ethylene glycol monoisopropyl ether	*see* 2-(1-Methylethoxy)ethanol
Ethylene glycol monophenyl ether	*see* 2-Phenoxyethanol
Ethylene glycol monopropyl ether	*see* 2-Propoxyethanol
Ethyleneimine	*see* Aziridine
Ethylenenaphthalene	*see* Acenaphthene
Ethylene oxide	*see* Oxirane
Ethyl ester acetoacetic acid	*see* Ethyl ester 3-oxobutanoic acid
Ethyl ester benzenepropanoic acid	*see* Ethyl benzenepropanoate
Ethyl ester benzoic acid	*see* Ethyl benzoate
Ethyl ester carbamic acid	62-017
Ethyl ester carbanilic acid	*see* Ethyl ester phenylcarbamic acid
Ethyl ester chloroacetic acid	*see* Ethyl chloroacetate
Ethyl ester 2-chloropropanoic acid	*see* Ethyl 2-chloropropanoate
Ethyl ester cyanoacetic acid	62-033
Ethyl ester cyclohexanecarboxylic acid	*see* Ethyl cyclohexanecarboxylate
Ethyl ester cyclopropanecarboxylic acid	*see* Ethyl cyclopropanecarboxylate
Ethyl ester dichloroacetic acid	*see* Ethyl dichloroacetate
Ethyl ester 2,3-dichloropropanoic acid	*see* Ethyl 2,3-dichloropropanoate
Ethyl ester 2,2-dimethylpropanoic acid	*see* Ethyl 2,2-dimethylpropanoate
S-Ethyl ester dipropylcarbamothionic acid	64-026
Ethyl ester nitric acid	*see* Ethyl nitrate
Ethyl ester 3-oxobutanoic acid	47-020
Ethyl ester phenylcarbamic acid	62-082
Ethyl ester 3-phenyl-2-propenoic acid	*see* Ethyl 3-phenyl-2-propenoate
Ethyl ester trichloroacetic acid	*see* Ethyl trichloroacetate
N-Ethylethanamide	*see N*-Ethylacetamide
N-Ethylethanamine	31-011
Ethyl ethanoate	*see* Ethyl acetate
Ethyl ether	*see* 1,1'-Oxybisethane
Ethyl formate	45-002
3-Ethylhexadecahydropyrene	12-106
Ethylhexahydroindan	*see* Ethyloctahydro-1*H*-indene
Ethyl hexanoate	45-056
2-Ethyl-1-hexanol	42-067
9-(2-Ethylhexyl)dodecahydrofluorene	12-119
9-(2-Ethylhexyl)perhydrofluorene	*see* 9-(2-Ethylhexyl)dodecahydrofluorene
Ethylhydrindan (unspecified isomer)	*see* Ethyloctahydro-1*H*-indene
Ethyl hydrocinnamate	*see* Ethyl benzenepropanoate
2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	42-049
1,1'-Ethylidenebisbenzene	14-073
1,1'-Ethylidenebiscyclohexane	12-091
1,1'-[Ethylidenebis(oxy)]bisbutane	41-043
Ethylidene chloride	*see* 1,1-Dichloroethane
Ethylidenecyclohexane	12-022

Ethylidenecyclopentane	12-011
Ethyl iodide	*see* Iodoethane
Ethylisobutylmethane	*see* 2-Methylhexane
Ethyl isobutyrate	*see* Ethyl 2-methylpropanoate
Ethyl isothiocyanate	*see* Isothiocyanatoethane
Ethyl isovalerate	*see* Ethyl 3-methylbutanoate
Ethyl mercaptan	*see* Ethanethiol
Ethyl methanoate	*see* Ethyl formate
2-(Ethylmethylamino)ethanol	62-041
Ethyl 3-methylbutanoate	45-041
N-Ethyl-*N*-methylethanamine	31-017
N, *N*-Ethylmethylethanolamine	*see* 2-(Ethylmethylamino)ethanol
Ethyl methyl ketone	*see* 2-Butanone
Ethyl methyl ketoxime (unspecified stereoisomer)	*see* 2-Butanone oxime
3-Ethyl-2-methylpentane	11-028
Ethyl-4-methylphenyl ether	*see* 1-Ethoxy-4-mythylbenzene
Ethyl 2-methylpropanoate	45-030
Ethyl methyl sulfide	*see* (Methylthio)ethane
Ethyl nitrate	62-008
Ethyloctahydro-1*H*-indene	12-061
Ethyl oxide	*see* 1,1'-Oxybisethane
Ethyloxirane	46-008
Ethyl 3-oxobutanoate	*see* Ethyl ester 3-oxobutanoic acid
3-Ethylpentane	11-020
Ethyl pentanoate	45-042
3-Ethyl-3-pentanol	42-062
Ethyl *tert*-pentyl ether	*see* 2-Ethoxy-2-methylbutane
2-Ethylperhydrophenanthrene	*see* 2-Ethyltetradecahydrophenanthrene
3-Ethylperhydropyrene	*see* 3-Ethylhexadecahydropyrene
Ethyl phenylcarbamate	*see* Ethyl ester phenylcarbamic acid
1-(4-Ethylphenyl)ethanone	43-046
Ethyl phenyl ether	*see* Ethoxybenzene
Ethyl phenyl ketone	*see* 1-Phenyl-1-propanone
Ethyl 3-phenylpropanoate	*see* Ethyl benzenepropanoate
Ethyl 3-phenyl-2-propenoate	45-086
Ethyl pivalate	*see* Ethyl 2,2-dimethylpropanoate
Ethyl propanoate	45-013
1-Ethyl-1-propanol	*see* 3-Pentanol
Ethyl propionate	*see* Ethyl propanoate
Ethyl propionyl	*see* 3-Pentanone
Ethyl propyl carbinol	*see* 3-Hexanol
Ethyl propyl ether	*see* 1-Ethoxypropane
Ethyl propyl ketone	*see* 3-Hexanone
Ethyl propyl sulfide	*see* 1-(Ethylthio)propane
2-Ethyltetradecahydrophenanthrene	12-099
N-Ethyl-*N*,2,4,6-tetranitrobenzenamine	62-074
Ethyltetryl	*see* *N*-Ethyl-*N*,2,4,6-tetranitrobenzenamine
1-(Ethylthio)propane	51-008
Ethyl *p*-tolyl ether	*see* 1-Ethoxy-4-methylbenzene
Ethyl trichloroacetate	61-017
Ethyl urethane	*see* Ethyl ester carbamic acid
Ethyl valerate	*see* Ethyl pentanoate
1,1'-(1,2-Ethynediyl)bisbenzene	14-067
Ethynylbenzene	14-015
Eugenol	*see* 2-Methoxy-4-(2-propenyl)phenol
Ferrocene	73-028
Fluoranthene	14-078
9*H*-Fluorene	14-061
Fluorine	01-008

Indium	01-016
Indium bromide (InBr)	02-017
Iodine	01-015
Iodine chloride	02-035
Iodine fluoride (IF_5)	02-067
Iodine monochloride	*see* Iodine chloride
Iodine pentafluoride	*see* Iodine fluoride (IF_5)
Iodobenzene	24-009
Iodoethane	24-003
Iodomethane	24-002
1-Iodo-3-methylbutane	24-006
1-Iodo-2-methylpropane	24-005
1-Iodopropane	24-004
β-Ionone	*see* 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
ψ-Ionone	*see* 6,10-Dimethyl-3,5,9-undecatriene-2-one
Isoamyl acetate	*see* 3-Methylbutyl acetate
Isoamyl alcohol	*see* 3-Methyl-1-butanol
sec-Isoamyl alcohol	*see* 3-Methyl-2-butanol
Isoamyl bromide	*see* 1-Bromo-3-methylbutane
Isoamyl butyrate	*see* 3-Methylbutyl butanoate
Isoamyl chloride	*see* 1-Chloro-3-methylbutane
α-Isoamylene	*see* 3-Methyl-1-butene
β-Isoamylene	*see* 2-Methyl-2-butene
Isoamyl formate	*see* 3-Methylbutyl formate
Isoamyl iodide	*see* 1-Iodo-3-methylbutane
Isoamyl isobutyrate	*see* 3-Methylbutyl 2-methylpropanoate
Isoamyl mercaptan	*see* 3-Methyl-1-butanethiol
sec-Isoamyl mercaptan	*see* 3-Methyl-2-butanethiol
Isoamyl propionate	*see* 3-Methylbutyl propanoate
Isoamyl valerate	*see* 3-Methylbutyl pentanoate
Isobutane	*see* 2-Methylpropane
Isobutanolamine	*see* 2-Amino-2-methyl-1-propanol
Isobutene	*see* 2-Methyl-1-propene
Isobutoxyethylene	*see* 1-(Ethenyloxy)-2-methylpropane
Isobutyl acetate	*see* 2-Methylpropyl acetate
Isobutyl alcohol	*see* 2-Methyl-1-propanol
Isobutylamine	*see* 2-Methyl-1-propanamine
Isobutyl bromide	*see* 1-Bromo-2-methylpropane
Isobutyl butyrate	*see* 2-Methylpropyl butanoate
Isobutyl chloride	*see* 1-Chloro-2-methylpropane
α-Isobutyldecalin	*see* Decahydro-1-(2-methylpropyl)naphthalene
Isobutyl formate	*see* 2-Methylpropyl formate
Isobutyl iodide	*see* 1-Iodo-2-methylpropane
Isobutyl isobutyrate	*see* 2-Methylpropyl 2-methylpropanoate
Isobutyl mercaptan	*see* 2-Methyl-1-propanethiol
Isobutyl methyl ketone	*see* 4-Methyl-2-pentanone
Isobutyl propionate	*see* 2-Methylpropyl propanoate
Isobutyl valerate	*see* 2-Methylpropyl pentanoate
Isobutyl vinyl ether	*see* 1-(Ethenyloxy)-2-methylpropane
Isobutyric acid	*see* 2-Methylpropanoic acid
Isobutyronitrile	*see* 2-Methylpropanenitrile
Isobutyryl chloride	*see* 2-Methylpropanoyl chloride
Isochroman	*see* 3,4-Dihydro-1*H*-2-benzopyran
1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene	62-093
1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene	62-094
Isodecane	*see* 2-Methylnonane
Isodurene	*see* 1,2,3,5-Tetramethylbenzene
Isoheptane	*see* 2-Methylhexane
Isooctane	*see* 2,2,4-Trimethylpentane

Isopentane	*see* 2-Methylbutane
Isopentyl acetate	*see* 3-Methylbutyl acetate
Isopentyl alcohol	*see* 3-Methyl-1-butanol
Isopentyl butyrate	*see* 3-Methylbutyl butanoate
Isopentyl formate	*see* 3-Methylbutyl formate
Isopentyl isobutyrate	*see* 3-Methylbutyl 2-methylpropanoate
Isopentyl mercaptan	*see* 3-Methyl-1-butanethiol
Isopentyl propionate	*see* 3-Methylbutyl propanoate
Isopentyl valerate	*see* 3-Methylbutyl pentanoate
Isophytol	*see* 3,7,11,15-Tetramethyl-1-hexadecen-3-ol
Isoprene	*see* 2-Methyl-1,3-butadiene
Isopropenylbenzene	*see* (1-Methylethenyl)benzene
m-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid	*see* 1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzen
p-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid	*see* 1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzen
Isopropenyl methyl ether	*see* 2-Methoxy-1-propene
2-Isopropoxyethanol	*see* 2-(1-Methylethoxy)ethanol
N-Isopropylacetamide	*see* *N*-(1-Methylethyl)acetamide
Isopropyl acetate	*see* 1-Methylethyl acetate
Isopropyl alcohol	*see* 2-Propanol
Isopropylamine	*see* 2-Propanamine
Isopropylbenzene	*see* (1-Methylethyl)benzene
Isopropylbicyclohexyl	*see* (1-Methylethyl)-1,1'-bicyclohexyl
Isopropylbiphenyl	*see* (1-Methylethyl)-1,1'-biphenyl
Isopropyl bromide	*see* 2-Bromopropane
Isopropyl cyanide	*see* 2-Methylpropanenitrile
Isopropylcyclohexylcyclohexane (unspecified isomer and stereoisomer)	*see* (1-Methylethyl)-1,1'-bicyclohexyl
Isopropyldecalin (unspecified isomer)	*see* Decahydro(1-methylethyl)naphthalene
α-Isopropyldecalin	*see* Decahydro-1-(1-methylethyl)naphthalene
Isopropyldiphenyl (unspecified isomer)	*see* (1-Methylethyl)-1,1'-biphenyl
Isopropylethylene	*see* 3-Methyl-1-butene
Isopropylhydrindan (unspecified isomer)	*see* Octahydro(1-methylethyl)-1*H*-indene
Isopropylidene chloride	*see* 2,2-Dichloropropane
4,4'-Isopropylidenediphenol	*see* 4,4'-(1-Methylethylidene)bisphenol
1-Isopropylidene-4-methylcyclohexan-2-on	*see* 5-Methyl-2-(1-methylethylidene)cyclohexanone
Isopropyl mercaptan	*see* 2-Propanethiol
1-Isopropyl-4-methylbenzene	*see* 1-Methyl-4-(1-methylethyl)benzene
Isopropyl methyl ether	*see* 2-Methoxypropane
Isopropyl methyl ketone	*see* 3-Methyl-2-butanone
7-Isopropyl-1-methylphenanthrene	*see* 1-Methyl-7-(1-methylethyl)phenanthrene
5-Isopropyl-2-methylphenol	*see* 2-Methyl-5-(1-methylethyl)phenol
Isopropyl methyl sulfide	*see* 2-(Methylthio)propane
Isopropyl nitrate	*see* 1-Methylethyl ester nitric acid
Isopropyltrimethylmethane	*see* 2,2,3-Trimethylbutane
Isoquinoline	33-036
Isothiocyanatobenzene	64-024
Isothiocyanatoethane	64-005
3-Isothiocyanato-1-propene	64-008
Isovaleric acid	*see* 3-Methylbutanoic acid
Isoxazole	62-010
Kalium	*see* Potassium
Ketohexamethylene	*see* Cyclohexanone
Krypton	01-018
Lactic acid (racemic)	*see* (*R,S*)-2-Hydroxypropanoic acid
Lauric acid	*see* Dodecanoic acid
Lauryl alcohol	*see* 1-Dodecanol
Lead(II) caprate	*see* Lead(2+) salt decanoic acid
Lead(II) caproate	*see* Lead(2+) salt hexanoic acid

Lead(II) caprylate	*see* Lead(2+) salt octanoic acid
Lead(II) decanoate	*see* Lead(2+) salt decanoic acid
Lead(II) dodecanoate	*see* Lead(2+) salt dodecanoic acid
Lead(II) hexadecanoate	*see* Lead(2+) salt hexadecanoic acid
Lead(II) hexanoate	*see* Lead(2+) salt hexanoic acid
Lead(II) laurate	*see* Lead(2+) salt dodecanoic acid
Lead(II) myristate	*see* Lead(2+) salt tetradecanoic acid
Lead(II) octadecanoate	*see* Lead(2+) salt octadecanoic acid
Lead(II) octanoate	*see* Lead(2+) salt octanoic acid
Lead(II) palmitate	*see* Lead(2+) salt hexadecanoic acid
Lead(2+) salt decanoic acid	74-009
Lead(2+) salt dodecanoic acid	74-012
Lead(2+) salt hexadecanoic acid	74-019
Lead(2+) salt hexanoic acid	74-004
Lead(2+) salt octadecanoic acid	74-022
Lead(2+) salt octanoic acid	74-006
Lead(2+) salt tetradecanoic acid	74-016
Lead(II) stearate	*see* Lead(2+) salt octadecanoic acid
Lead(II) tetradecanoate	*see* Lead(2+) salt tetradecanoic acid
Limonene	*see* 1-Methyl-4-(1-methylethenyl)cyclohexene
Linalol	*see* 3,7-Dimethyl-1,6-octadien-3-ol
Lithium	01-019
Lithium nitrate	*see* Lithium salt nitric acid
Lithium salt nitric acid	02-096
2,3-Lutidine	*see* 2,3-Dimethylpyridine
2,4-Lutidine	*see* 2,4-Dimethylpyridine
2,5-Lutidine	*see* 2,5-Dimethylpyridine
2,6-Lutidine	*see* 2,6-Dimethylpyridine
3,4-Lutidine	*see* 3,4-Dimethylpyridine
3,5-Lutidine	*see* 3,5-Dimethylpyridine
Maleic anhydride	*see* 2,5-Furandione
Malononitrile	*see* Propanedinitrile
D-Mannitol	42-050
Margaric acid	*see* Heptadecanoic acid
MBBA	*see* 4-Butyl-*N*-[(4-methoxyphenyl)methylene]benzenamine
Mellitene	*see* Hexamethylbenzene
p-Menth-4(8)-en-3-one	*see* 5-Methyl-2-(1-methylethylidene)cyclohexanone
3-Mercaptopropanoic acid	63-003
Mercury	01-014
Mercury(II) caprate	*see* Mercury(2+) salt decanoic acid
Mercury(II) caprylate	*see* Mercury(2+) salt octanoic acid
Mercury(II) decanoate	*see* Mercury(2+) salt decanoic acid
Mercury(II) dodecanoate	*see* Mercury(2+) salt dodecanoic acid
Mercury(II) hexadecanoate	*see* Mercury(2+) salt hexadecanoic acid
Mercury iodide (HgI_2)	02-094
Mercury(II) laurate	*see* Mercury(2+) salt dodecanoic acid
Mercury(II) myristate	*see* Mercury(2+) salt tetradecanoic acid
Mercury(II) octadecanoate	*see* Mercury(2+) salt octadecanoic acid
Mercury(II) octanoate	*see* Mercury(2+) salt octanoic acid
Mercury(II) palmitate	*see* Mercury(2+) salt hexadecanoic acid
Mercury(2+) salt decanoic acid	74-008
Mercury(2+) salt dodecanoic acid	74-011
Mercury(2+) salt hexadecanoic acid	74-018
Mercury(2+) salt octadecanoic acid	74-021
Mercury(2+) salt octanoic acid	74-005
Mercury(2+) salt tetradecanoic acid	74-015
Mercury(II) stearate	*see* Mercury(2+) salt octadecanoic acid
Mercury(II) tetradecanoate	*see* Mercury(2+) salt tetradecanoic acid
Mesitylene	*see* 1,3,5-Trimethylbenzene

1-Methylcyclohexanol	42-056
2-Methylcyclohexanol	42-057
cis-2-Methylcyclohexanol	42-058
trans-2-Methylcyclohexanol	42-059
3-Methylcyclohexanol	42-060
4-Methylcyclohexanol	42-061
m-Methylcyclohexanone	*see* 3-Methylcyclohexanone
o-Methylcyclohexanone	*see* 2-Methylcyclohexanone
p-Methylcyclohexanone	*see* 4-Methylcyclohexanone
2-Methylcyclohexanone	43-026
3-Methylcyclohexanone	43-027
4-Methylcyclohexanone	43-028
4-Methylcyclohexene	14-014
3-Methyl-4-cyclohexene-1,2-dicarboxylic acid anhydride	*see* 3a,4,7,7a-Tetrahydro-4-methyl-1,3-isobenzofurandione
1-Methylcyclohexylcyclohexane	*see* 2-Methyl-1,1'-bicyclohexyl
Methylcyclopentane	12-008
1-Methylcyclopentene	14-007
3-Methylcyclopentene	14-008
2-Methylcyclothiapentane	*see* 2-Methyltetrahydrothiophene
3-Methylcyclothiapentane	*see* 3-Methyltetrahydrothiophene
α-Methyldecalin	*see* Decahydro-1-methylnaphthalene
β-Methyldecalin	*see* Decahydro-2-methylnaphthalene
2-Methyldecane	11-047
Methyl decanoate	45-089
Methyl dichloroacetate	61-011
N-Methyldiethylamine	*see* *N*-Ethyl-*N*-methylethanamine
Methyl 2,4-dimethylphenyl ether	*see* 1-Methoxy-2,4-dimethylbenzene
Methyl 2,2-dimethylpropanoate	45-031
2-Methyl-1,3-dinitrobenzene	62-066
6-Methyl-5,7-dioxaundecane	*see* 1,1'-[Ethylidenebis(oxy)]bisbutane
4-Methyl-1,3-dioxolan-2-one	47-007
N-Methyldiphenylamine	*see* *N*-Methyl-*N*-phenylbenzenamine
Methyldipropylmethane	*see* 4-Methylheptane
Methyl diselenide	*see* Dimethyl diselenide
Methyl disulfide	*see* 2,3-Dithiabutane
Methyl enanthoate	*see* Methyl heptanoate
4,4'-Methylenebisbenzenamine	31-044
1,1'-Methylenebisbenzene	14-062
1,1'-Methylenebiscyclohexane	12-076
1,1'-Methylenebis[4-isocyanatobenzene]	62-099
Methylenebis[trimethylsilane]	71-019
Methylene bromide	*see* Dibromomethane
Methylene chloride	*see* Dichloromethane
Methylenecyclobutane	12-003
3-Methylenecyclobutanecarbonitrile	32-018
3-Methylenecyclobutyl cyanide	*see* 3-Methylenecyclobutanecarbonitrile
Methylenecyclohexane	12-012
4,4'-Methylenedianiline	*see* 4,4'-Methylenebisbenzenamine
1,1'-(Methylenedi-4,1-phenylene)bis-1*H*-pyrrole-2,5-dione	62-116
Methylenedi-*p*-phenylene ester isocyanic acid	*see* 1,1'-Methylenebis[4-isocyanatobenzene]
Methylene iodide	*see* Diiodomethane
4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane	12-046
Methyl ester benzoic acid	*see* Methyl benzoate
Methyl ester bicyclo[1.1.0]butane-1-carboxylic acid	*see* Methyl bicyclo[1.1.0]butane-1-carboxylate
Methyl ester carbanilic acid	*see* Methyl ester phenylcarbamic acid
Methyl ester chloroacetic acid	*see* Methyl chloroacetate
Methyl ester cyclobutanecarboxylic acid	*see* Methyl cyclobutanecarboxylate
Methyl ester dichloroacetic acid	*see* Methyl dichloroacetate
Methyl ester 2,2-dimethylpropanoic acid	*see* Methyl 2,2-dimethylpropanoate

p-Nitrotoluene	*see* 1-Methyl-4-nitrobenzene
1-Nitro-3-(trifluoromethyl)benzene	64-022
Nitrous oxide	*see* Nitrogen oxide (N_2O)
Nonadecane	11-058
Nonadecanoic acid	44-035
Nonadecylic acid	*see* Nonadecanoic acid
Nonanal	43-044
Nonane	11-038
Nonanoic acid	44-023
1-Nonanol	42-084
5-Nonanone	43-045
1-Nonene	13-034
Nonyl acrylate	*see* Nonyl 2-propenoate
Nonyl alcohol	*see* 1-Nonanol
Nonyl aldehyde	*see* Nonanal
4-Nonyl-1,1'-bicyclohexyl	12-121
n-Nonyl bromide	*see* 1-Bromononane
4-Nonylcyclohexylcyclohexane	*see* 4-Nonyl-1,1'-bicyclohexyl
Nonyl ester carbanilic acid	*see* Nonyl phenylcarbamate
Nonyl ester 2-methyl-2-propenoic acid	*see* Nonyl 2-methyl-2-propenoate
Nonyl ester phenylcarbamic acid	*see* Nonyl phenylcarbamate
Nonyl ester 2-propenoic acid	*see* Nonyl 2-propenoate
Nonyl methacrylate	*see* Nonyl 2-methyl-2-propenoate
Nonyl 2-methyl-2-propenoate	45-099
Nonyl phenylcarbamate	62-103
Nonyl 2-propenoate	45-093
4'-Nonyl-1,1':3',1''-tercyclohexane	12-123
4-Nonyl-*m*-tercyclohexyl	*see* 4'-Nonyl-1,1':3',1''-tercyclohexane
Nopinene	*see* 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane
2,5-Norbornadiene	*see* Bicyclo[2.2.1]hepta-2,5-diene
endo-2-Norbornanecarbonitrile	*see endo*-Bicyclo[2.2.1]heptane-2-carbonitrile
exo-2-Norbornanecarbonitrile	*see exo*-Bicyclo[2.2.1]heptane-2-carbonitrile
Norcarane	*see* Bicyclo[4.1.0]heptane
Octacosane	11-068
cis-Octadecafluorodecahydronaphthalene	21-031
trans-Octadecafluorodecahydronaphthalene	21-032
Octadecafluorooctane	21-029
Octadecane	11-057
Octadecanoic acid	44-034
1-Octadecanol	42-103
(*Z*)-9-Octadecenoic acid	44-033
Octadecyl alcohol	*see* 1-Octadecanol
Octaethylcyclotetrasiloxane	71-042
Octafluorocyclobutane	21-007
Octafluoropropane	21-006
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1,2,3,4,5,6,7,8-Octahydroanthracene	14-074
Octahydroazocine	33-030
Octahydro-1*H*-indene	12-039
cis-Octahydro-1*H*-indene	12-040
trans-Octahydro-1*H*-indene	12-041
Octahydro-4,7-methano-1*H*-indene	12-047
Octahydro(1-methylethyl)-1*H*-indene	12-070
Octahydromethyl-1*H*-indene	12-053
cis-Octahydropentalene	12-025
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2,2,4,4,6,6,8,8-Octamethylcyclotetrasilazane	71-024
Octamethylcyclotetrasiloxane	71-023
Octamethyldiphenylcyclopentasiloxane (unspecified isomer)	71-048

Ozone	01-024
Palmitic acid	*see* Hexadecanoic acid
Paraldehyde	*see* 2,4,6-Trimethyl-1,3,5-trioxane
Pelargonic acid	*see* Nonanoic acid
Pelargonic aldehyde	*see* Nonanal
Pentaborane (9)	02-012
Pentacene	14-090
Pentachloroethane	22-007
Pentacontane	11-083
Pentacosane	11-065
Pentadecane	11-053
Pentadecanoic acid	44-030
1-Pentadecanol	42-101
Pentadecanolactone	*see* Oxacyclohexadecan-2-one
Pentadecanolide	*see* Oxacyclohexadecan-2-one
2-Pentadecanone	43-061
n-Pentadecyl alcohol	*see* 1-Pentadecanol
Pentadecylic acid	*see* Pentadecanoic acid
1,2-Pentadiene	13-013
cis-1,3-Pentadiene	*see* (*Z*)-1,3-Pentadiene
(*E*)-1,3-Pentadiene	13-014
trans-1,3-Pentadiene	*see* (*E*)-1,3-Pentadiene
(*Z*)-1,3-Pentadiene	13-015
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2,3-Pentadiene	13-017
Pentaerythrityl tetrabromide	*see* 1,3-Dibromo-2,2-bis(bromomethyl)propane
Pentaerythrityl tetrachloride	*see* 1,3-Dichloro-2,2-bis(chloromethyl)propane
Pentaerythrityl tetrafluoride	*see* 1,3-Difluoro-2,2-bis(fluoromethyl)propane
Pentaethylene glycol	*see* 3,6,9,12-Tetraoxatetradecane-1,14-diol
Pentafluoroaniline	*see* 2,3,4,5,6-Pentafluorobenzenamine
2,3,4,5,6-Pentafluorobenzenamine	64-014
Pentafluorobenzene	21-012
1,1,2,2,2-Pentafluoro-*N*, *N*-bis(pentafluoroethyl)ethanamine	64-013
Pentafluoromethylbenzene	21-023
Pentafluoronitrobenzene	64-012
1,1,2,2,2-Pentafluoro-*N*-(pentafluoroethyl)-*N*-(trifluoromethyl)-ethanamine	64-011
Pentafluorophenol	61-034
2,3,4,5,6-Pentafluorotoluene	*see* Pentafluoromethylbenzene
Pentafluoro(trifluoromethyl)benzene	21-020
Pentalin	*see* Pentachloroethane
Pentamethylbenzene	14-049
Pentamethylene	*see* Cyclopentane
Pentamethylene dichloride	*see* 1,5-Dichloropentane
Pentamethylene oxide	*see* Tetrahydropyran
Pentamethylene sulfide	*see* Tetrahydro-2*H*-thiopyran
Pentamethylenimine	*see* Piperidine
2,2,4,6,6-Pentamethylheptane	11-050
Pentanal	43-012
1-Pentanamine	31-018
Pentane	11-010
Pentanedinitrile	32-013
1,5-Pentanediol	42-033
2,4-Pentanedione	43-009
Pentanenitrile	32-016
1-Pentanethiol	52-013
Pentanoic acid	44-012
1-Pentanol	42-029
2-Pentanol	42-030

3-Pentanol	42-031
5-Pentanolide	*see* Tetrahydro-2*H*-pyran-2-one
2-Pentanone	43-013
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1,4,7,10,13-Pentaoxacyclopentadecane	46-025
2,5,8,11,14-Pentaoxapentadecane	41-044
Pentatriacontane	11-076
1-Pentene	13-021
2-Pentene	13-022
cis-2-Pentene	*see* (*Z*)-2-Pentene
(*E*)-2-Pentene	13-023
trans-2-Pentene	*see* (*E*)-2-Pentene
(*Z*)-2-Pentene	13-024
Pentoxane	*see* 1,3,5,7,9-Pentoxecane
1,3,5,7,9-Pentoxecane	46-016
Pentyl acetate	45-045
tert-Pentyl alcohol	*see* 2-Methyl-2-butanol
Pentyl aldehyde	*see* Pentanal
Pentylamine	*see* 1-Pentanamine
Pentyl butanoate	45-074
Pentyl butyrate	*see* Pentyl butanoate
Pentylene glycol dimethyl ether	*see* 1,5-Dimethoxypentane
Pentyl ethanoate	*see* Pentyl acetate
1-Pentyl mercaptan	*see* 1-Pentanethiol
2-Pentyl-2-nonenal	43-059
N-*p*-*n*-Pentyloxybenzylidene-*p*'-*n*-butylaniline	*see* 4-Butyl-*N*-[[4-(pentyloxy)phenyl]methylene]-benzenamine
Pentyl propanoate	45-062
Perbromomethane	*see* Tetrabromomethane
Perchloric acid	02-034
Perchloroethylene	*see* Tetrachloroethene
Perchloromethane	*see* Tetrachloromethane
Perchloryl fluoride ($(ClO_3)F$)	02-031
Perfluoroacetone	*see* 1,1,1,3,3,3-Hexafluoro-2-propanone
Perfluorobenzene	*see* Hexafluorobenzene
Perfluorobiphenyl	*see* 2,2',3,3',4,4',5,5',6,6'-Decafluoro-1,1'-biphenyl
Perfluoro-3-butyltetrahydrofuran	*see* 2,2,3,3,4,5,5-Heptafluorotetrahydro-4-(nonafluorobutyl)furan
Perfluorocyclobutane	*see* Octafluorocyclobutane
cis-Perfluorodecaline	*see cis*-Octadecafluorodecahydronaphthalene
trans-Perfluorodecaline	*see trans*-Octadecafluorodecahydronaphthalene
Perfluorodimethylcyclohexane	*see* Decafluorobis(trifluoromethyl)cyclohexane
Perfluoroethane	*see* Hexafluoroethane
Perfluoroethylene	*see* Tetrafluoroethene
Perfluoroheptane	*see* Hexadecafluoroheptane
Perfluorohexane	*see* Tetradecafluorohexane
Perfluoromethane	*see* Tetrafluoromethane
Perfluoromethylcyclohexane	*see* (Trifluoromethyl)undecafluorocyclohexane
Perfluorooctane	*see* Octadecafluorooctane
Perfluoropentane	*see* Dodecafluoropentane
Perfluoropiperidine	*see* Undecafluoropiperidine
Perfluoropropane	*see* Octafluoropropane
Perfluorotoluene	*see* Pentafluoro(trifluoromethyl)benzene
Perhydroazepine	*see* Hexahydro-1*H*-azepine
Perhydroazine	*see* Piperidine
Perhydroazocine	*see* Octahydroazocine
cis-Perhydroazulene	*see cis*-Decahydroazulene
Perhydro-1,4-diazine	*see* Piperazine

cis-syn-trans-Perhydrophenantrene	*see* (4aα,4bα,8aα,10aβ)-Tetradecahydrophenanthrene
trans-anti-cis-Perhydrophenanthrene	*see* (4aα,4bβ,8aα,10aα)-Tetradecahydrophenanthrene
trans-anti-trans-Perhydrophenanthrene	*see* (4aα,4bβ,8aα,10aβ)-Tetradecahydrophenanthrene
Perylene	14-087
Phenanthrene	14-068
Phenanthridine	33-044
Phenethyl alcohol	*see* Benzeneethanol
Phenethylamine	*see* Benzeneethanamine
Phenetole	*see* Ethoxybenzene
Phenol	42-034
2-Phenoxyethanol	47-030
(Phenoxymethyl)oxirane	47-036
Phenylacetylene	*see* Ethynylbenzene
Phenylamine	*see* Benzenamine
N-Phenylbenzenamine	31-042
Phenyl bromide	*see* Bromobenzene
1-Phenylbutane	*see* Butylbenzene
2-Phenylbutane	*see* (1-Methylpropyl)benzene
Phenyl chloride	*see* Chlorobenzene
Phenyl cyanide	*see* Benzonitrile
Phenylcyclohexane	*see* Cyclohexylbenzene
1,3-Phenylenediamine	*see* 1,3-Benzenediamine
Phenyl ester 2-hydroxybenzoic acid	47-041
Phenyl ester isothiocyanic acid	*see* Isothiocyanatobenzene
Phenylethane	*see* Ethylbenzene
2-Phenylethanol	*see* Benzeneethanol
1-Phenylethanone	43-036
2-Phenylethylamine	*see* Benzeneethanamine
Phenylethyl carbinol	*see* Benzenepropanol
Phenylformic acid	*see* Benzoic acid
Phenyl glycidyl ether	*see* (Phenoxymethyl)oxirane
11-Phenylheneicosane	14-096
11-Phenylhenicosane	*see* 11-Phenylheneicosane
1-Phenylheptane	*see* Heptylbenzene
1-Phenylhexane	*see* Hexylbenzene
Phenylhydrazine	34-007
Phenylhydrazone acetaldehyde	34-009
Phenyl mercaptan	*see* Benzenethiol
Phenyl methane	*see* Methylbenzene
Phenylmethyl acetate	45-065
Phenylmethylamine	*see* Benzenemethanamine
Phenylmethyl ester acetic acid	*see* Phenylmethyl acetate
Phenylmethyl ester 2-methyl-2-propenoic acid	*see* Phenylmethyl 2-methyl-2-propenoate
Phenylmethyl 2-methyl-2-propenoate	45-087
1-Phenyloctane	*see* Octylbenzene
3-Phenyl-1-propanol	*see* Benzenepropanol
1-Phenyl-1-propanone	43-041
3-Phenyl-2-propenal	43-040
3-Phenylpropylamine	*see* Benzenepropanamine
Phenyl propyl ether	*see* Propoxybenzene
Phenyl salicylate	*see* Phenyl ester 2-hydroxybenzoic acid
Phenyl sulfide	*see* 1,1'-Thiobisbenzene
5'-Phenyl-1,1':3',1''-terphenyl	14-091
Phenyl *m*-tolyl ketone	*see* (3-Methylphenyl)phenylmethanone
Phosgene	*see* Carbonic dichloride
Phosphine	02-088
Phosphoric acid	02-087
Phosphorous fluoride (PF_3)	*see* Phosphorous trifluoride
Phosphorous trichloride	02-044

R12	*see* Dichlorodifluoromethane
R13	*see* Chlorotrifluoromethane
R13B1	*see* Bromotrifluoromethane
R14	*see* Tetrafluoromethane
R21	*see* Dichlorofluoromethane
R22	*see* Chlorodifluoromethane
R23	*see* Trifluoromethane
R112	*see* 1,1,2,2-Tetrachloro-1,2-difluoroethane
R113	*see* 1,1,2-Trichloro-1,2,2-trifluoroethane
R114	*see* 1,2-Dichloro-1,1,2,2-tetrafluoroethane
R114B2	*see* 1,2-Dibromo-1,1,2,2-tetrafluoroethane
R115	*see* Chloropentafluoroethane
R122	*see* 1,1,2-Trichloro-1,2-difluoroethane
R132	*see* 1,1-Dichloro-1,2-difluoroethane
R142	*see* 1-Chloro-1,1-difluoroethane
Resorcinol	*see* 1,3-Benzenediol
Retene	*see* 1-Methyl-7-(1-methylethyl)phenanthrene
Rubidium	01-026
Rubidium fluoride ($Rb(HF_2)$)	02-059
Rubidium hydrogen difluoride	*see* Rubidium fluoride ($Rb(HF_2)$)
Sabinene	*see* 4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane
Salicyl aldehyde	*see* 2-Hydroxybenzaldehyde
Salicylic acid	*see* 2-Hydroxybenzoic acid
Salol	*see* Phenyl ester 2-hydroxybenzoic acid
Selenium	01-028
β-Selenium diglycol	*see* 2,2'-Selenodiethanol
Selenobismethane	73-002
2,2'-Selenodiethanol	73-009
Silane	02-090
Silicon chloride	*see* Tetrachlorosilane
Silver nitrate	*see* Silver(1+) salt nitric acid
Silver(1+) salt nitric acid	02-001
Sodium	01-021
Sodium butanoate	*see* Sodium salt butanoic acid
Sodium chlorate	*see* Sodium salt chloric acid
Sodium formate	*see* Sodium salt formic acid
Sodium propanoate	*see* Sodium salt propanoic acid
Sodium salt butanoic acid	74-003
Sodium salt chloric acid	02-036
Sodium salt formic acid	74-001
Sodium salt propanoic acid	74-002
Spirocyclane	*see* Spiropentane
Spiropentane	12-004
Squalane	*see* 2,6,10,15,19,23-Hexamethyltetracosane
Stannane	*see* Tin
Stannic iodide	*see* Tetraiodostannane
Stearic acid	*see* Octadecanoic acid
Stearyl alcohol	*see* 1-Octadecanol
Stilbene	*see* (*E*)-1,1'-(1,2-Ethenediyl)bisbenzene
Styrene	*see* Ethenylbenzene
Suberone	*see* Cycloheptanone
Succinimide	*see* 2,5-Pyrrolidinedione
Succinonitrile	*see* Butanedinitrile
Sulfinylbismethane	63-001
Sulfolane	*see* Tetrahydrothiophene 1,1-dioxide
4,4'-Sulfonylbisbenzenamine	64-028
1,1'-Sulfonylbis(4-chlorobenzene)	64-027
Sulfonylbismethane	63-002
4,4'-Sulfonyldianiline	*see* 4,4'-Sulfonylbisbenzenamine

1,1,2-Tribromoethane	23-016
1,1,2-Tribromoethane-1-*d*	23-011
1,1,2-Tribromoethane-2-*d*	23-012
1,1,2-Tribromoethane-2,2-d_2	23-008
1,1,2-Tribromoethane-1,2,2-d_3	23-006
Tribromomethane	23-002
1,2,3-Tribromopropane	23-020
Tributyrin	*see* 1,2,3-Propanetriyl tributanoate
Tricaproin	*see* 1,2,3-Propanetriyl ester hexanoic acid
Trichloroacetaldehyde	61-003
Trichloroacetic acid	61-004
1,2,4-Trichlorobenzene	22-035
2,2,3-Trichlorobutanal	61-016
2,2,3-Trichlorobutyraldehyde	*see* 2,2,3-Trichlorobutanal
1,1,2-Trichloro-1,2-difluoroethane	25-018
Trichloroethanal	*see* Trichloroacetaldehyde
β-Trichloroethane	*see* 1,1,2-Trichloroethane
1,1,1-Trichloroethane	22-015
1,1,2-Trichloroethane	22-016
Trichloroethanoic acid	*see* Trichloroacetic acid
Trichloroethene	22-006
Trichloroethenylsilane	71-001
Trichloroethylene	*see* Trichloroethene
Tri(2-chloroethyl)phosphate	*see* 2-Chloroethanol phosphate (3:1)
Trichloroethylsilane	71-002
Trichlorofluoromethane	25-005
Trichloromethane	22-002
Trichlorophenylsilane	71-011
1,2,3-Trichloropropane	22-022
Trichlorosilane	02-042
o-Trichlorosilanediphenyl	*see* [1,1'-Biphenyl]-2-yltrichlorosilane
p-Trichlorosilanediphenyl	*see* [1,1'-Biphenyl]-4-yltrichlorosilane
o-(Trichlorosilyl)biphenyl	*see* [1,1'-Biphenyl]-2-yltrichlorosilane
p-(Trichlorosilyl)biphenyl	*see* [1,1'-Biphenyl]-4-yltrichlorosilane
3-Trichlorosilylpropanenitrile	71-004
1,3,5-Trichloro-2,4,6-trifluorobenzene	25-030
1,1,1-Trichloro-2,2,2-trifluoroethane	25-013
1,1,2-Trichloro-1,2,2-trifluoroethane	25-014
1,1,1-Trichloro-3,3,3-trifluoropropane	25-023
Trichlorovinylsilane	*see* Trichloroethenylsilane
Tricosane	11-063
Tricresyl phosphate	*see* Tris(methylphenyl) ester phosphoric acid
Tricyclo[5.2.1.$0^{2,6}$]decane	*see* Octahydro-4,7-methano-1*H*-indene
Tricyclo[3.3.2.$0^{2,8}$]deca-3,6,9-triene	14-034
Tricyclo[6.2.1.$1^{3,6}$]dodecane	12-064
1,1,3-Tricyclohexylpropane	*see* 1,1',1''-(1-Propanyl-2-ylidene)triscyclohexane
Tridecane	11-051
Tridecanoic acid	44-028
Tridecanoin	*see* 1,2,3-Propanetriyl ester decanoic acid
1-Tridecanol	42-097
Tridecanolactone	*see* Oxacyclotetradecan-2-one
Tridecanolide	*see* Oxacyclotetradecan-2-one
n-Tridecyl alcohol	*see* 1-Tridecanol
Tridecylic acid	*see* Tridecanoic acid
Trideuterated ammonia	*see* Ammonia-d_3
Trideuteroglycerol	*see* 1,2,3-Propanetriol-*O*, *O*, *O*-d_3
Triethanolamine	*see* 2,2',2''-Nitrilotrisethanol
Triethanolamine borate	*see* 2,8,9-Trioxa-5-aza-1-borabicyclo[3.3.3]undecane
Triethoxymethane	*see* 1,1',1''-[Methylidynetris(oxy)]trisethane

3-(Triethoxysilyl)-1-propanamine	71-026
3-(Triethoxysilyl)propylamine	*see* 3-(Triethoxysilyl)-1-propanamine
Triethylaluminium	73-018
Triethylamine	*see* *N*, *N*-Diethylethanamine
Triethylamineborane	72-010
Triethylantimony	*see* Triethylstibine
Triethylarsine	73-019
Triethylbismuthine	73-020
Triethylborane	72-009
Triethylenediamine	*see* 1,4-Diazobicyclo[2.2.2]octane
Triethylene glycol	*see* 2,2'-[1,2-Ethanediylbis(oxy)]bisethanol
Triethylene glycol dimethyl ether	*see* 2,5,8,11-Tetraoxadodecane
Triethylenetetramine	*see* *N*, *N*'-Bis(2-aminoethyl)-1,2-ethanediamine
Triethyl ester orthoformic acid	*see* 1,1',1''-[Methylidynetris(oxy)]trisethane
Triethylgallium	73-021
Triethylindium	73-022
Triethylmethane	*see* 3-Ethylpentane
Triethyl orthoformate	*see* 1,1',1''-[Methylidynetris(oxy)]trisethane
Triethylstibine	73-023
Trifluoroacetonitrile	64-003
Trifluoroacetyl fluoride	61-002
Trifluoroborane	02-008
1,1,1-Trifluoroethane	21-005
Trifluoroethanenitrile	*see* Trifluoroacetonitrile
2,2,2-Trifluoroethanol	61-008
Trifluoromethane	21-002
Trifluoromethanethiol	64-002
(Trifluoromethyl)benzene	21-024
Trifluoromethyl cyanide	*see* Trifluoroacetonitrile
m-Trifluoromethylnitrobenzene	*see* 1-Nitro-3-(trifluoromethyl)benzene
(Trifluoromethyl)undecafluorocyclohexane	21-021
α,α,α-Trifluorotoluene	*see* (Trifluoromethyl)benzene
Triglyme	*see* 2,5,8,11-Tetraoxadodecane
Trihexanoin	*see* 1,2,3-Propanetriyl ester hexanoic acid
N, *N*, *N*-Trihexyl-1-hexanaminium perchlorate	74-013
Tri(2-hydroxyethyl)amine	*see* 2,2',2''-Nitrilotrisethanol
Trilaurin	*see* 1,2,3-Propanetriyl ester dodecanoic acid
Trimellitic anhydride	*see* 1,3-Dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid
Trimethylacetaldehyde	*see* 2,2-Dimethylpropanal
Trimethylacetonitrile	*see* 2,2-Dimethylpropanenitrile
1,3,5-Trimethyladamantane	*see* 1,3,5-Trimethyltricyclo[3.3.1.$1^{3,7}$]decane
Trimethylaluminium	73-005
Trimethylamine	*see* *N*, *N*-Dimethylmethanamine
Trimethylamineborane	72-006
Trimethylarsine	73-006
N, *N*, 2-Trimethylbenzenamine	31-038
1,2,3-Trimethylbenzene	14-030
1,2,4-Trimethylbenzene	14-031
1,3,5-Trimethylbenzene	14-032
2,6,6-Trimethylbicyclo[3.1.1]heptane	12-054
1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one	*see* Camphor
Trimethylborane	72-005
2,2,3-Trimethylbutane	11-024
Trimethyl carbinol	*see* 2-Methyl-2-propanol
2,5,6-Trimethyl-2-cyclohexen-1-one	43-042
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	43-054
3,7,11-Trimethyl-1-dodecyn-3-ol	42-100
Trimethylene	*see* Cyclopropane
Trimethylene bromide	*see* 1,3-Dibromopropane

Trimethylene dichloride	*see* 1,3-Dichloropropane
Trimethylenedicyanide	*see* Pentanedinitrile
Trimethylene oxide	*see* Oxetane
Trimethylene sulfide	*see* Thietane
Trimethylethylene	*see* 2-Methyl-2-butene
Trimethylgallium	73-007
Trimethylhydrazine	34-005
Trimethylmethane	*see* 2-Methylpropane
Trimethylolpropane	*see* 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol
6,10,14-Trimethyl-3,5-pentadecadien-2-one	43-063
6,10,14-Trimethyl-2-pentadecanone	43-064
2,2,4-Trimethylpentane	11-034
2,3,3-Trimethylpentane	11-035
2,3,4-Trimethylpentane	11-036
2,4,4-Trimethyl-1-pentene	13-032
2,4,4-Trimethyl-2-pentene	13-033
2,3,6-Trimethylpyridine	33-031
2,4,6-Trimethylpyridine	33-032
1-[2-(Trimethylsilyl)ethyl]azetidine	71-020
1-[2-(Trimethylsilyl)ethyl]aziridine	71-043
N-[(β-Trimethylsilyl)ethyl]ethylenimine	*see* 1-[2-(Trimethylsilyl)ethyl]aziridine
N-(β-Trimethylsilylethyl)trimethylenimine	*see* 1-[2-(Trimethylsilyl)ethyl]azetidine
1,3,5-Trimethyltricyclo[3.3.1.1^{3,7}]decane	12-071
2,4,6-Trimethyl-1,3,5-trioxane	46-018
cis-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	*see* (2α,4α,6α)-2,4,6-Trimethyl-2,4,6-triphenyl-cyclotrisiloxane
trans-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	*see* (2α,4α,6β)-2,4,6-Trimethyl-2,4,6-triphenyl-cyclotrisiloxane
(2α,4α,6α)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	71-049
(2α,4α,6β)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	71-050
Trimethylvinylsilane	*see* Ethenyltrimethylsilane
Trimyristin	*see* 1,2,3-Propanetriyl ester tetradecanoic acid
1,3,5-Tri-α-naphthylbenzene	*see* 1,1',1''-(1,3,5-Benzenetriyl)trisnaphthalene
2,4,6-Trinitro-*N*-(methylnitro)-*m*-toluidine	*see* 3-Methyl-2,4,6-trinitro-*N*-(nitromethyl)benzenamine
Trinitrophenylethylnitroamine	*see* *N*-Ethyl-*N*,2,4,6-tetranitrobenzenamine
Trinitrophenylmethylnitroamine	*see* *N*-Methyl-2,4,6-tetranitrobenzenamine
2,4,6-Trinitrotoluene	*see* 2-Methyl-1,3,5-trinitrobenzene
Trioctanoin	*see* 1,2,3-Propanetriyl ester octanoic acid
2,8,9-Trioxa-5-aza-1-borabicyclo[3.3.3]undecane	72-007
sym-Trioxane	*see* 1,3,5-Trioxane
1,3,5-Trioxane	46-005
2,5,8-Trioxanonane	*see* 1,1'-Oxybis(2-methoxyethane)
3,6,9-Trioxaundecane	*see* 1,1'-Oxybis(2-ethoxyethane)
Tripalmitin	*see* 1,2,3-Propanetriyl ester hexadecanoic acid
1,3,5-Triphenylbenzene	*see* 5'-Phenyl-1,1':3',1''-terphenyl
Triphenylene	14-080
Triphenyl ester phosphoric acid	72-013
Triphenylmethane	*see* 1,1',1''-Methylidynetrisbenzene
Triphenyl phosphate	*see* Triphenyl ester phosphoric acid
Triphenylphosphine oxide	72-012
Tripropionin	*see* 1,2,3-Propanetriyl tripropanoate
Tripropylaluminium	73-027
Triptane	*see* 2,2,3-Trimethylbutane
Triptycene	*see* 9,10-Dihydro-9,10[1',2']-benzenoanthracene
1,1,1-Tris(hydroxymethyl)propane	*see* 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol
Tris(methylphenyl) ester phosphoric acid	72-014
Tristearin	*see* 1,2,3-Propanetriyl ester octadecanoic acid
Tritane	*see* 1,1',1''-Methylidynetrisbenzene
Tritetracontane	11-080

Trithiocarbonic acid	02-023
Tritol	*see* 2-Methyl-1,3,5-trinitrobenzene
Tritolyl phosphate (unspecified isomer)	*see* Tris(methylphenyl) ester phosphoric acid
Tritriacontane	11-074
Trometamol	*see* 2-Amino-2-(hydroxymethyl)-1,3-propanediol
Unatriacontane	*see* Hentriacontane
Undecafluoropiperidine	64-010
Undecane	11-048
Undecanoic acid	44-026
1-Undecanol	42-094
Undecanolactone	*see* Oxacyclododecan-2-one
Undecanolide	*see* Oxacyclododecan-2-one
α-Undecene	*see* 1-Undecene
1-Undecene	13-036
Undecyl alcohol	*see* 1-Undecanol
Undecylic acid	*see* Undecanoic acid
Uranium(VI) fluoride	02-071
Uranium hexafluoride	*see* Uranium(VI) fluoride
Urea	62-004
USAN	*see* 2-Oxetanone
Valeraldehyde	*see* Pentanal
Valeric acid	*see* Pentanoic acid
δ-Valerolactam	*see* 2-Piperidinone
δ-Valerolactone	*see* Tetrahydro-2*H*-pyran-2-one
Valeronitrile	*see* Pentanenitrile
Valeryl chloride	*see* Pentanoyl chloride
Vinegar acid	*see* Acetic acid
Vinyl acetate	*see* Ethenyl acetate
Vinylbenzene	*see* Ethenylbenzene
Vinyl bromide	*see* Bromoethene
Vinyl chloride	*see* Chloroethene
Vinyl cyanide	*see* 2-Propenenitrile
Vinylethylene	*see* 1,3-Butadiene
Vinylidene chloride	*see* 1,1-Dichloroethene
Vinyl trichloride	*see* 1,1,2-Trichloroethane
Water	02-075
Water-d_2	02-053
Wood alcohol	*see* Methanol
Wood ether	*see* Oxybismethane
Xenon	01-030
m-Xylene	*see* 1,3-Dimethylbenzene
o-Xylene	*see* 1,2-Dimethylbenzene
p-Xylene	*see* 1,4-Dimethylbenzene
2,6-Xylidine	*see* 2,6-Dimethylbenzenamine

0. Inorganic Substances

01. Elements

The elements family contains 30 members that have melting temperatures below 573 K which is the upper temperature limit for including a compound in this monograph. All measurements of the 30 elements were performed over a range of temperatures.

For the sake of clarity, this introduction is subdivided into several parts, each covering one group of elements depending on their physical state at ambient temperature (gases, liquids and solids). Measurements on these elements were carried out in diverse laboratories by various experimental techniques which differed largely because of their individual properties and unique characteristics.

Gaseous elements, hydrogen, deuterium, nitrogen, oxygen, and rare gases, were measured mainly before World War II in German laboratories at TUB, UMG, UWG (16EUC, 28EUC/HAU, 29CLU2, 29CLU/HIL, 35CLU/BAR, 36CLU, 38CLU/KRU, 38CLU/RIC) and in USA at UCB (29GIA/JOH, 33GIA/CLA). Ortho-deuterium and para-hydrogen were measured after World War II at OSU (50JOH/CLA, 51KER/RIF). Some of the elements have never been reinvestigated since, and therefore, the above measurements served in most cases as a basis for the final correlation. This was particularly the case for all of the rare gases (except helium, see below). Regarding more recent sources, extensive data sets from NBSB were published for para-hydrogen (62YOU/DIL), nitrogen (81WEB, 91MAG), and oxygen (69GOO/WEB). These data were measured in an adiabatic spherical calorimeter (61GOO) up to the critical region with an estimated uncertainty of 0.3 to 0.7 % (the higher value applies to the vicinity of the critical point) and were preferred in the correlation to the older sources. The latter data have been, however, considered in certain cases when they were consistent with the NBSB data.

Interpreting the experimental data for two isotopes of helium (^{3}He and ^{4}He) was outside the scope of this monograph. Liquid helium exists only over a very narrow temperature range and a sharp λ-transition requires special treatment as part of the correlation which would not be consistent with the approach used for other compounds. We have, therefore, presented only a survey of the main data sources for the heat capacity of helium in this compilation.

The four halogen elements exist at ambient temperature in three different phases (fluorine and chlorine are gases, bromine is a liquid, and iodine is a solid). Very extensive and reliable measurements of fluorine are available from NBSB (70GOO/PRY) with data covering the entire range of temperatures up to the critical temperature. Data for chlorine from UCB (39GIA/POW) have been preferred to older and less accurate data from TUB (24EUC/KAR). Only one data set, measured at DCM (58HIL/KRA), is available for bromine. Two data sets were available for iodine; the older but apparently more reliable source (37CAR/HAR) has been selected. All halogens exhibit a minimum on the heat capacity curve just below the normal boiling temperature. This phenomenon is frequently observed for chemical elements and is discussed in a more general manner in the literature (93ZAB/BUR).

Liquid heat capacity data are available in addition for two non-metallic elements, phosphorus and sulfur, which are solids at ambient temperature. Only smoothed data presented as parameters of a quadratic equation are available for liquid phosphorus from UCB (42YOU/HIL) in the temperature range from 298 to 370 K. This equation partly describes the undercooled liquid for which the lower temperature limit is almost 20 K below the melting temperature. Certain properties of sulfur, such as the enthalpy of fusion, melting temperature and heat capacity, are very sensitive to impurities in the sample. Five available sets of experimental data differ significantly from each other and we have selected the values originating from the publication presenting the combined measurements in three Austrian laboratories and one American laboratory (73KOM/MIL) using a single sample of highest purity. The heat capacity curve $C_p = f(T)$ exhibits a sharp maximum around 435 K that is due to the decay of the eight-member S_8 ring into a linear chain. In order to avoid the anomalous heat capacity values caused by this sharp transition, we have divided the entire temperature interval into two subintervals. The lower temperature subinterval covers the range from the melting temperature to 432.15 K and the other subinterval from 438.15 K to 598.15 K; data in each subinterval were correlated by a separate polynomial.

The last part of this introduction deals with solid metallic elements. Most metals have melting temperatures high above ambient temperature and the interval between the melting and normal boiling temperature is generally large. Heat capacity of liquid metals usually decreases slowly with temperature or data remain constant within the experimental error over a wide temperature interval. For that reason, most data for many metals were calculated from measurements which were carried out in high temperature drop calorimeters under extreme temperature conditions. In those cases, when the data reached into the temperature region of our interest (melting temperature below 573 K), we have frequently taken the data recommended in the monograph by Hultgren (63HUL/ORR) as well as data supplemented with more recent references.

Mercury, gallium, and alkali metals have melting temperatures substantially lower than most other metals, however, their $C_p = f(T)$ curve is similar to that for other metals. Three reliable and consistent data sets have been selected for correlating heat capacity of mercury: an extensive data set from NBSW (51DOU/BAL), additional data sets from UCB (53BUS/GIA), and data from IICN (79AMI/LEB). In the case of gallium, data by (83TAK/KAD) measured jointly at two Japanese laboratories and measurements from ICCN (84AMI/MIN) have been selected as the most reliable. Alkali metals were studied systematically at NBSW; data have been selected for lithium (55DOU/EPS) (a joint research effort with Knolls Atomic Laboratory, Schenectady, New York), sodium (50GIN/DOU) and potassium (52DOU/BAL) with uncertainties between 0.3 and 0.4 %. Parameters of a linear smoothing equation are available for rubidium (13REN), however, for cesium only two data points were measured (55DAU/MAR).

Name: Argon
Formula: Ar

CAS–RN: 7440–37–1
Group No.: 1–001
Molar Mass: 39.95

TABLE 1.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
16EUC	84.9–93.9	5	nosp	not specified		C_{sat}	BSIO	16EUC
28EUC/HAU	90.0–140.0	6S	nosp	not specified		C_{sat}	BSIO	28EUC/HAU
36CLU	86.6–88.9	3	nosp	not specified		C_{sat}	BSIO	36CLU/GOL
61FLU/LEA	84.6–86.3	3	0.50	99.9997	melpt	C_p	BSAO	61FLU/LEA

TABLE 1.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
16EUC	84.9–93.9	5	3.00#	1.086	1.74–1	3.26	–1.50–1	–3
28EUC/HAU	90.0–140.0	6	2.00#	1.254	1.54–1	2.51	–2.73–2	0
61FLU/LEA	84.6–86.3	3	0.50	2.860	7.78–2	1.43	1.42–2	–1
				Rejected data				
36CLU	(3.51–1, 6.91, –3.49–1, –3)							

TABLE 1.1.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	12	0.744	8.14–2	1.26	–5.32–3	–1
C_{sat}	17	12	0.492	3.96–2	0.69	–6.60–3	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
84.6–105.0	5.21208+1	–1.50242+2	1.57885+2	–5.41279+1	V
105.0–140.0	–1.28816+2	3.66722+2	–3.34461+2	1.02172+2	V
84.6–110.0	2.05119+1	–4.98369+1	5.23003+1	–1.74277+1	V
110.0–140.0	–9.06124+1	2.53229+2	–2.23214+2	6.60616+1	V

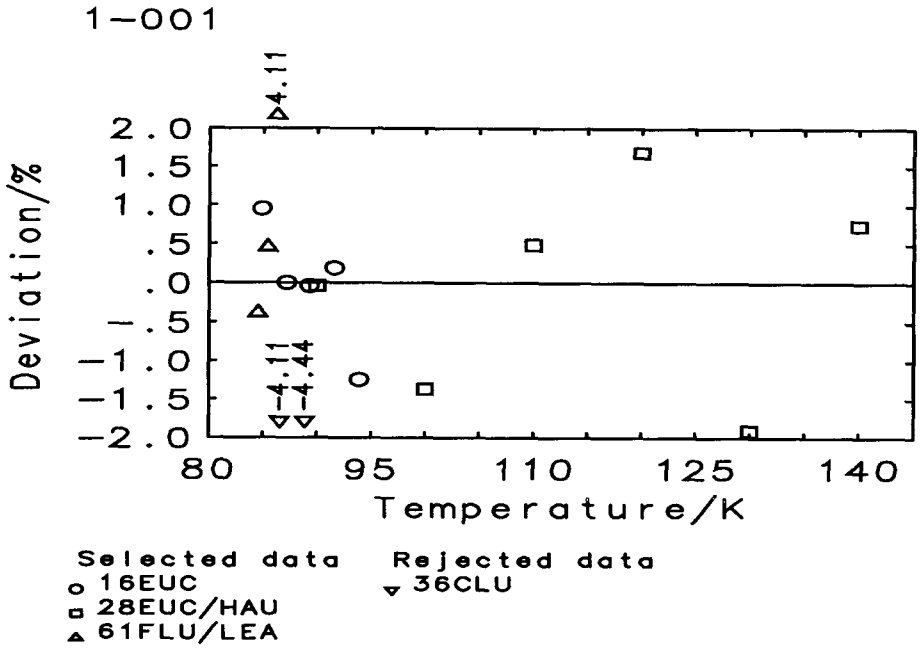
TABLE 1.1.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140
c_p (J K^{-1}g^{-1})	1.11	1.17	1.22	1.29	1.49	1.96
C_p (J K^{-1}mol^{-1})	44.3	46.9	48.8	51.4	59.5	78.2
c_{sat} (J K^{-1}g^{-1})	1.11	1.15	1.20	1.25	1.35	1.60
C_{sat} (J K^{-1}mol^{-1})	44.2	46.1	48.0	49.8	54.0	63.9

TABLE 1.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	12	0.871	6.54–2	1.12	1.15–2	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
84.6–140.0	150.80	1.03253–1	3.75540–1	4.50207	7.09719–3	V



Name: Bismuth
Formula: Bi

CAS-RN: 7440-69-9
Group No.: 1-002
Molar Mass: 208.98

TABLE 1.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
26AWB/GRI	N	543.2–673.2	2	nosp	not specified	C_p	DSIO	26AWB/GRI
26UMI		573.2–873.2	5S	nosp	99.875 anal	C_{avg}	not specified	
32CAR/HAR		545.6–644.1	10	0.50	99.986 anal	C_p	BSIO	30CAR/STO
40KUB/SCH	N	548.2–798.2	2	nosp	not specified	C_{avg}	DSIO	40KUB/SCH
71BEL/HUL		544.8–801.8	21	nosp	99.9999 anal	C_p	DSIO	71BEL/HUL
83JOA/PAL	N	544.5	1	nosp	not specified	C_p	not specified	

26AWB/GRI constant value calculated from temperature dependence of enthalpy by the authors; suspect value
40KUB/SCH constant value calculated from temperature dependence of enthalpy by the authors; suspect value
83JOA/PAL the origin of data unclear

TABLE 1.2.2. Correlated heat capacities

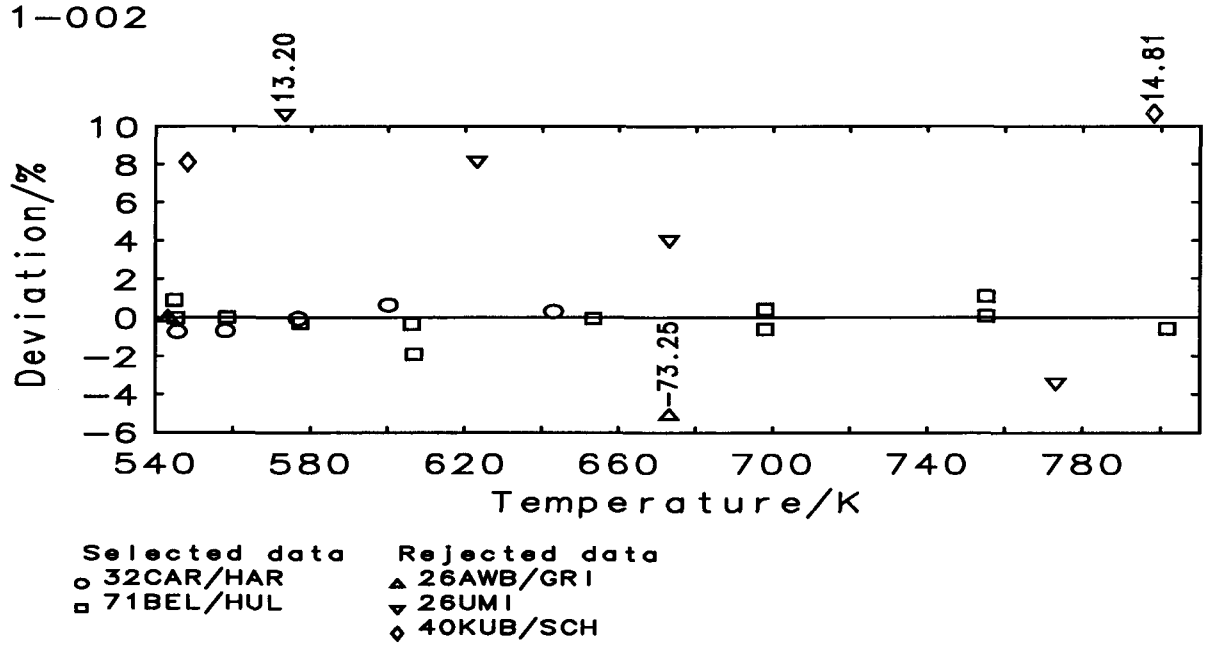
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
32CAR/HAR	545.6–644.1	10	0.50	1.202	2.16–2	0.60	−1.48–3	0
71BEL/HUL	544.8–801.8	21	0.50#	1.263	2.23–2	0.63	−1.11–3	−2
				Rejected data				
26AWB/GRI	(1.46, 73.25, −1.46, −1)			26UMI	(3.29–1, 8.20, 2.24–1, 2)			
40KUB/SCH	(4.75–1, 11.93, 4.55–1, 2)							

TABLE 1.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	31	1.308	2.32–2	0.65	2.77–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
544.8–801.8		5.87111	–6.09214–1	3.73303–2			IV

TABLE 1.2.4. Recommended values of heat capacities

Temp. (K)	550	570	590	610	630	650	670
c_p (J K^{-1}g^{-1})	0.145	0.144	0.142	0.141	0.140	0.139	0.138
C_p (J K^{-1}mol^{-1})	30.35	30.03	29.73	29.47	29.22	29.00	28.81
Temp. (K)	690	710	730	750	770	790	810
c_p (J K^{-1}g^{-1})	0.137	0.136	0.136	0.135	0.135	0.135	0.135
C_p (J K^{-1}mol^{-1})	28.64	28.50	28.38	28.28	28.22	28.17	28.15



Name: Bromine
Formula: Br_2

CAS–RN: 7726–95–6
Group No.: 1–003
Molar Mass: 159.81

TABLE 1.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
58HIL/KRA	265.9–300.0	6	nosp	99.999	melpt	C_p	BSAO	58HIL/KRA

TABLE 1.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.009	2.36–4	0.00	4.77–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
265.9–300.0		2.14218+1	−7.90841	1.26668			III

TABLE 1.3.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	0.484	0.482	0.479	0.476	0.474	0.473
C_p (J K^{-1}mol^{-1})	77.35	77.08	76.57	76.00	75.69	75.63

Name: Chlorine
Formula: Cl_2

CAS–RN: 7782–50–5
Group No.: 1–004
Molar Mass: 70.91

TABLE 1.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24EUC/KAR	187.7–197.0	6	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
39GIA/POW	179.0–236.8	11	nosp	99.997	melpt	C_p	BSIO	37GIA/EGA

TABLE 1.4.2. Correlated heat capacities

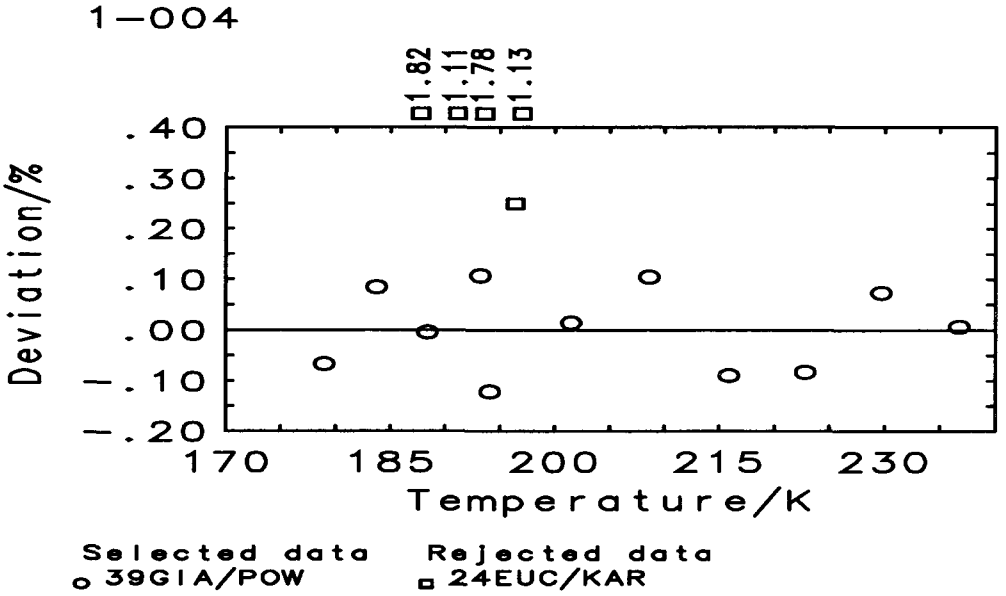
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
39GIA/POW	179.0–236.8	11	0.40#	0.199	6.37–3	0.08	1.01–5	1
				Rejected data				
24EUC/KAR	(1.57–1, 1.90, 1.32–1, 6)							

TABLE 1.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	17	11	0.233	7.46–3	0.09	1.01–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
179.0–236.8		7.69170	5.55367–1	−1.94679–1			III

TABLE 1.4.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	0.945	0.943	0.941	0.938	0.935	0.931
C_p (J K^{-1}mol^{-1})	67.02	66.88	66.71	66.51	66.28	66.01



Name: Cesium
Formula: Cs

CAS–RN: 7440–46–2
Group No.: 1–005
Molar Mass: 132.91

TABLE 1.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
13REN	302.0–373.0	eqn	nosp	not specified		C_p	DSIO	13REN
55DAU/MAR	310.0–320.0	2S	0.20	not specified		C_p	BSAO	55DAU/MAR

TABLE 1.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
55DAU/MAR	310.0–320.0	2	0.20	0.000	0.00	0.00	0.00	0
				Rejected data				
13REN	(1.17–1, 2.95, 1.17–1, 1)							

TABLE 1.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
310.0–320.0		3.83451					III

TABLE 1.5.4. Recommended values of heat capacities

Temp. (K)	310	320
c_p (J K^{-1}g^{-1})	0.240	0.240
C_p (J K^{-1}mol^{-1})	31.88	31.88

Name: Deuterium (D_2)
Formula: D_2

CAS-RN: 7782-39-0
Group No.: 1-006
Molar Mass: 4.03

TABLE 1.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
35CLU/BAR	N	19.4-21.7	8	nosp	99.7	estim	C_{sat}	BSIO	36CLU/GOL

35CLU/BAR content of HD 0.3 %

TABLE 1.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	8	8	0.611	1.56-2	0.61	1.41-4	1

Temp. range K	A_1	A_2	Level of uncertainty
19.4-21.7	3.23134-1	1.11682+1	IV

TABLE 1.6.4. Recommended values of heat capacities

Temp. (K)	19.50	20	20.50	21	21.50
c_{sat} (J K^{-1}g^{-1})	5.162	5.278	5.393	5.508	5.623
C_{sat} (J K^{-1}mol^{-1})	20.79	21.26	21.72	22.19	22.65

Name: *ortho*-Deuterium (D_2)
Formula: D_2

CAS-RN: 7782-39-0
Group No.: 1-007
Molar Mass: 4.03

TABLE 1.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51KER/RIF	N	19.9-22.7	8	nosp	99.2	anal	C_p	BSIO	50JOH/CLA

51KER/RIF sample contained 97.8 % *ortho*-Deuterium; C_p values were corrected for presence of HD (1.1 %)

TABLE 1.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	8	8	0.528	7.47-3	0.26	2.98-5	0

Temp. range K	A_1	A_2	Level of uncertainty
19.9-22.7	7.29466-1	1.01918+1	III

TABLE 1.7.4. Recommended values of heat capacities

Temp. (K)	20	20.50	21	21.50	22	22.50
c_p ($J K^{-1} g^{-1}$)	5.713	5.818	5.924	6.029	6.134	6.239
C_p ($J K^{-1} mol^{-1}$)	23.01	23.44	23.86	24.28	24.71	25.13

Name: Fluorine
Formula: F_2

CAS-RN: 7782-41-4
Group No.: 1-008
Molar Mass: 38.00

TABLE 1.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
37KAN	57.5–83.4	5	nosp	not specified		C_p	BSIO	37KAN
53HU/WHI2	58.1–81.3	6	nosp	99.97	melpt	C_p	BSIO	50JOH/CLA
70GOO/PRY	55.2–143.4	36	nosp	99.99	anal	C_{sat}	BSAO	61GOO

TABLE 1.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70GOO/PRY	55.2–140.7	34	0.30#	1.687	5.94–2	0.51	8.54–4	–2
				Rejected data				
37KAN	(1.21, 21.89, –1.21, –5)			53HU/WHI2	(1.46–1, 2.11, 1.20–1, 6)			

TABLE 1.8.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	47	34	1.894	6.67–2	0.57	8.54–4	–2
C_{sat}	47	34	1.330	4.05–2	0.40	3.40–4	–3

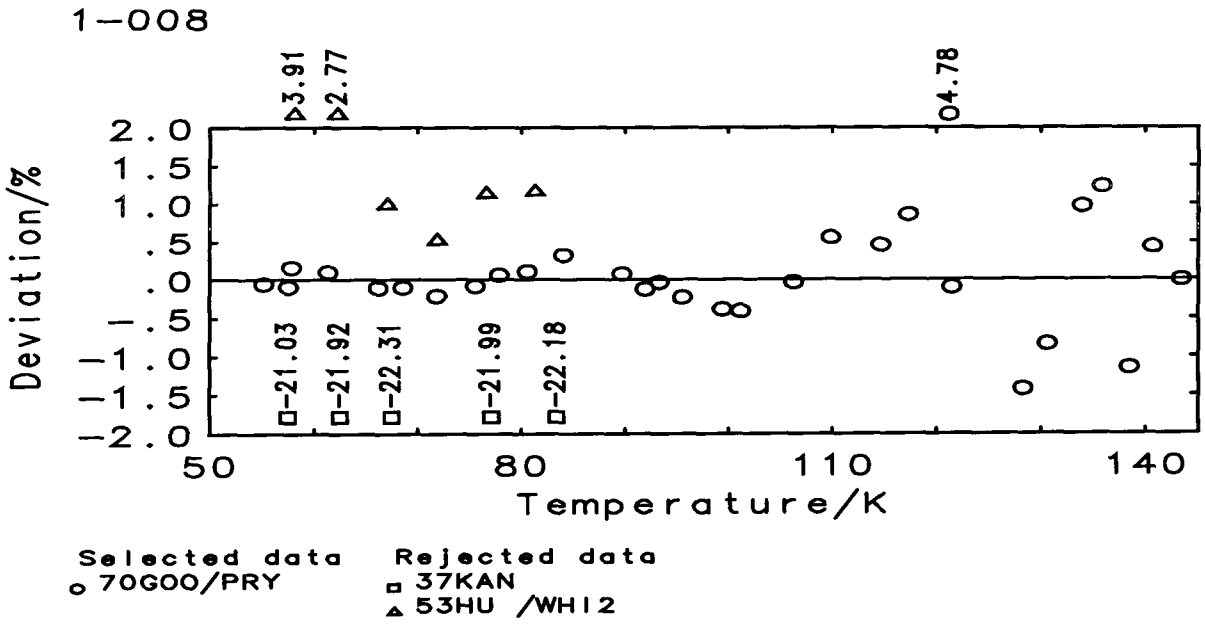
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
55.2–85.0	–2.66035	3.71743+1	–4.94806+1	2.23401+1	III
85.0–105. 0	1.48979+1	–2.47958+1	2.34254+1	–6.25044	III
105.0–132. 0	–1.30711+2	3.91230+2	–3.72789+2	1.19532+2	IV
132.0–140. 7	–2.00495+4	4.56611+4	–3.46682+4	8.77998+3	V
55.2–85.0	–1.67553	3.28266+1	–4.31301+1	1.92659+1	III
85.0–105.0	1.30737+1	–1.92295+1	1.81125+1	–4.75079	III
105.0–132.0	–8.11488+1	2.49978+2	–2.38275+2	7.66421+1	IV
132.0–140.7	–1.16463+4	2.65345+4	–2.01508+4	5.10505+3	V

TABLE 1.8.4. Recommended values of heat capacities

Temp. (K)	60	70	80	90	100	110	120
c_p ($J\,K^{-1}g^{-1}$)	1.457	1.483	1.499	1.532	1.592	1.677	1.860
C_p ($J\,K^{-1}mol^{-1}$)	55.35	56.36	56.95	58.20	60.50	63.72	70.67
c_{sat} ($J\,K^{-1}g^{-1}$)	1.456	1.483	1.498	1.526	1.577	1.646	1.782
C_{sat} ($J\,K^{-1}mol^{-1}$)	55.33	56.35	56.93	57.99	59.91	62.56	67.73
Temp. (K)	130	140					
c_p ($J\,K^{-1}g^{-1}$)	2.294	4.11					
C_p ($J\,K^{-1}mol^{-1}$)	87.18	156					
c_{sat} ($J\,K^{-1}g^{-1}$)	2.083	3.21					
C_{sat} ($J\,K^{-1}mol^{-1}$)	79.15	122					

TABLE 1.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	47	34	2.094	5.88–2	0.63	–1.47–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
55.2–140.7	144.30	–1.41175	2.83069–1	6.31565	–1.11994	–3.37656	2.28286	IV



Name: Gallium
Formula: Ga

CAS–RN: 7440–55–3
Group No.: 1–009
Molar Mass: 69.72

TABLE 1.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33ROT/MEY2	N	298.1–313.1	2	nosp	not specified		C_p	DSIO	33ROT/MEY2
34ROT/MEY	N	298.1–373.1	2S	nosp	not specified		C_{avg}	DSIO	33ROT/MEY2
52ADA/JOH		306.9–322.8	4	nosp	99.98	melpt	C_p	BSAO	52ADA/JOH
83TAK/KAD		298.3–613.4	87	1.00	99.9999	anal	C_p	BDHO	79TAK/YOK
84AMI/MIN		304.4–319.2	27	nosp	99.9999	anal	C_p	BSAO	79AMI/LEB

33ROT/MEY2 constant value calculated from temperature dependence of enthalpy by the authors; correct data in 34ROT/MEY
34ROT/MEY corrected data from 33ROT/MEY2; a constant value calculated from temperature dependence of enthalpy by the authors

TABLE 1.9.2. Correlated heat capacities

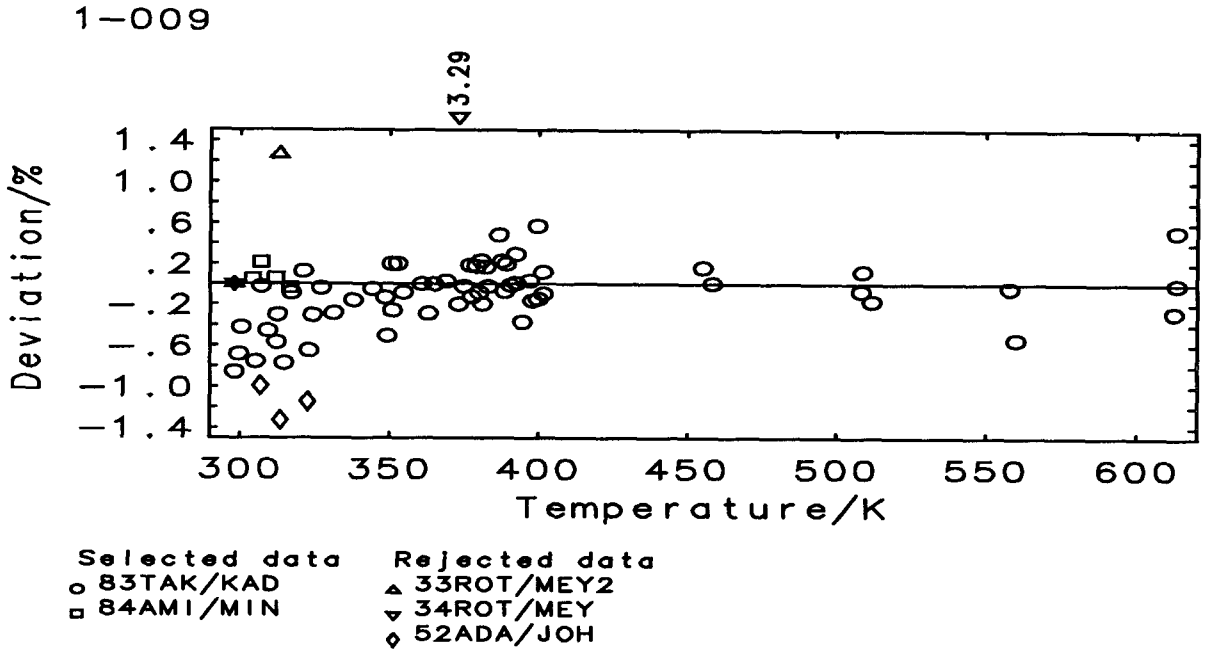
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83TAK/KAD	298.3–613.4	87	1.00	0.301	1.01–2	0.30	–3.71–3	–27
84AMI/MIN	304.4–319.2	27	0.30#	0.215	2.20–3	0.06	1.10–3	11
				Rejected data				
33ROT/MEY2	(4.34–2, 1.26, 4.34–2, 1)			34ROT/MEY	(1.13–1, 3.28, 1.13–1, 1)			
52ADA/JOH	(3.89–2, 1.16, –3.88–2, –4)							

TABLE 1.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	122	114	0.288	9.03–3	0.27	–2.57–3	–16
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
298.3–613.4		4.50213	–6.03882–1	9.73838–2	–5.57025–3		IV

TABLE 1.9.4. Recommended values of heat capacities

Temp. (K)	300	320	340	360	380	400	420
c_p (J K^{-1}g^{-1})	0.407	0.404	0.400	0.397	0.394	0.392	0.390
C_p (J K^{-1}mol^{-1})	28.41	28.14	27.90	27.69	27.50	27.34	27.20
Temp. (K)	440	460	480	500	520	540	560
c_p (J K^{-1}g^{-1})	0.388	0.387	0.385	0.384	0.383	0.382	0.381
C_p (J K^{-1}mol^{-1})	27.07	26.96	26.87	26.78	26.71	26.64	26.57
Temp. (K)	580	600					
c_p (J K^{-1}g^{-1})	0.380	0.379					
C_p (J K^{-1}mol^{-1})	26.51	26.45					



Name: Hydrogen
Formula: H_2

CAS-RN: 1333-74-0
Group No.: 1-010
Molar Mass: 2.02

TABLE 1.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
16EUC	17.4–21.3	5	nosp	not specified	C_{sat}	BSIO	16EUC
23SIM/LAN	15.4–18.6	8	nosp	not specified	C_{sat}	BSIO	23SIM/LAN

TABLE 1.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
16EUC	17.4–21.3	5	2.00#	0.937	4.11-2	1.87	2.00-2	3
23SIM/LAN	15.4–18.6	8	1.00#	0.777	1.55-2	0.78	-2.60-3	0

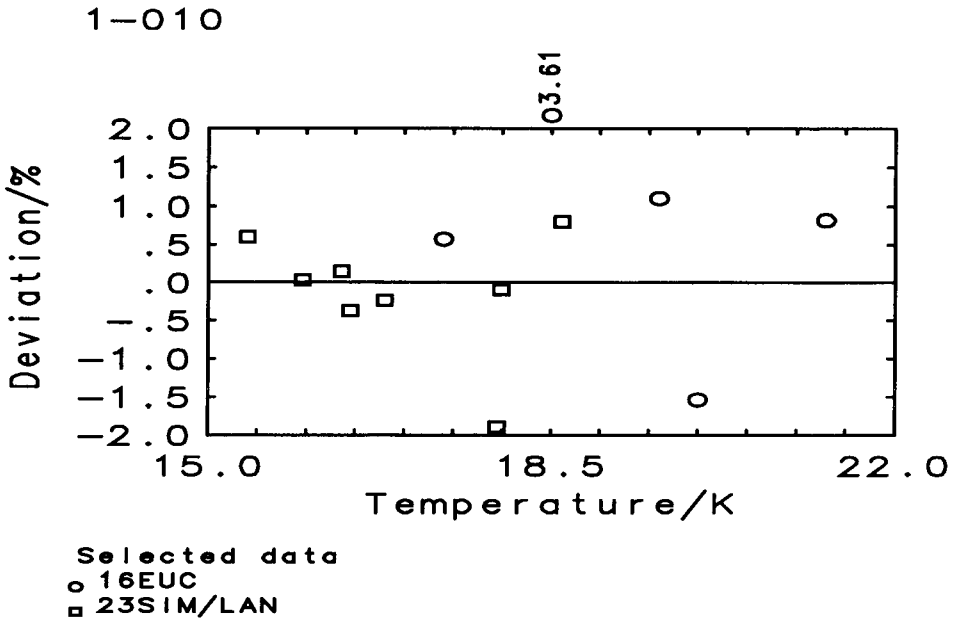
TABLE 1.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	13	13	0.916	3.07-2	1.43	6.08-3	3
C_{sat}	13	13	0.786	2.83-2	1.33	3.78-3	2

Temp. range K	A_1	A_2	Level of uncertainty
15.4–21.3	1.00111-1	1.07833+1	V
15.4–21.3	2.05678-1	1.01391+1	V

TABLE 1.10.4. Recommended values of heat capacities

Temp. (K)	15	17	19	21
c_p ($J\,K^{-1}g^{-1}$)	7.08	7.97	8.86	9.75
C_p ($J\,K^{-1}mol^{-1}$)	14.3	16.1	17.9	19.7
c_{sat} ($J\,K^{-1}g^{-1}$)	7.12	7.96	8.79	9.63
C_{sat} ($J\,K^{-1}mol^{-1}$)	14.4	16.0	17.7	19.4



Name: *para*-Hydrogen
Formula: H_2

CAS-RN: 1333-74-0
Group No.: 1-011
Molar Mass: 2.02

TABLE 1.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
29CLU/HIL	N	15.1–18.0	6	1.50	not specified	C_p	BSIO	29CLU1
50JOH/CLA	N	15.1–19.0	10	0.50	not specified	C_p	BSIO	50JOH/CLA
54SMI/HAL	N	18.3–31.5	8	1.00	99.79 anal	C_{sat}	BSIO	53RIF/KER
62YOU/DIL	N	14.8–31.5	32	0.30	99.99 estim	C_{sat}	BSAO	61GOO

29CLU/HIL sample contained 94.0 % *para*-Hydrogen
50JOH/CLA sample contained 99.8 % *para*-Hydrogen
54SMI/HAL sample contained 0.21 % *ortho*-Hydrogen
62YOU/DIL error increased near critical temperature

TABLE 1.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50JOH/CLA	16.3–19.0	7	0.50	1.635	1.64–2	0.82	–5.29–3	–3
62YOU/DIL	14.8–31.5	32	0.30	1.543	2.92–2	0.46	8.48–4	4
				Rejected data				
29CLU/HIL	(5.22–2, 2.83, 1.96–2, 2)			54SMI/HAL	(2.16–1, 3.06, 1.50–2, 0)			

TABLE 1.11.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	56	39	1.695	2.98–2	0.59	–2.54–4	1
C_{sat}	56	39	1.356	1.77–2	0.52	–5.30–4	–1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
14.8–21.0	1.70966	–1.43623+1	1.15069+2	–1.39395+2	III
21.0–28.0	1.88860+1	2.79861+2	–1.28599+3	2.08452+3	IV
28.0–31.5	–1.03753+3	1.11939+4	–4.02648+4	4.84879+4	V
14.8–21.0	1.84338–1	9.74303	–6.81781	5.38039+1	III
21.0–28.0	–1.15732+1	1.77709+2	–8.06654+2	1.32339+3	IV
28.0–31.5	–5.77711+2	6.24347+3	–2.24701+4	2.71132+4	V

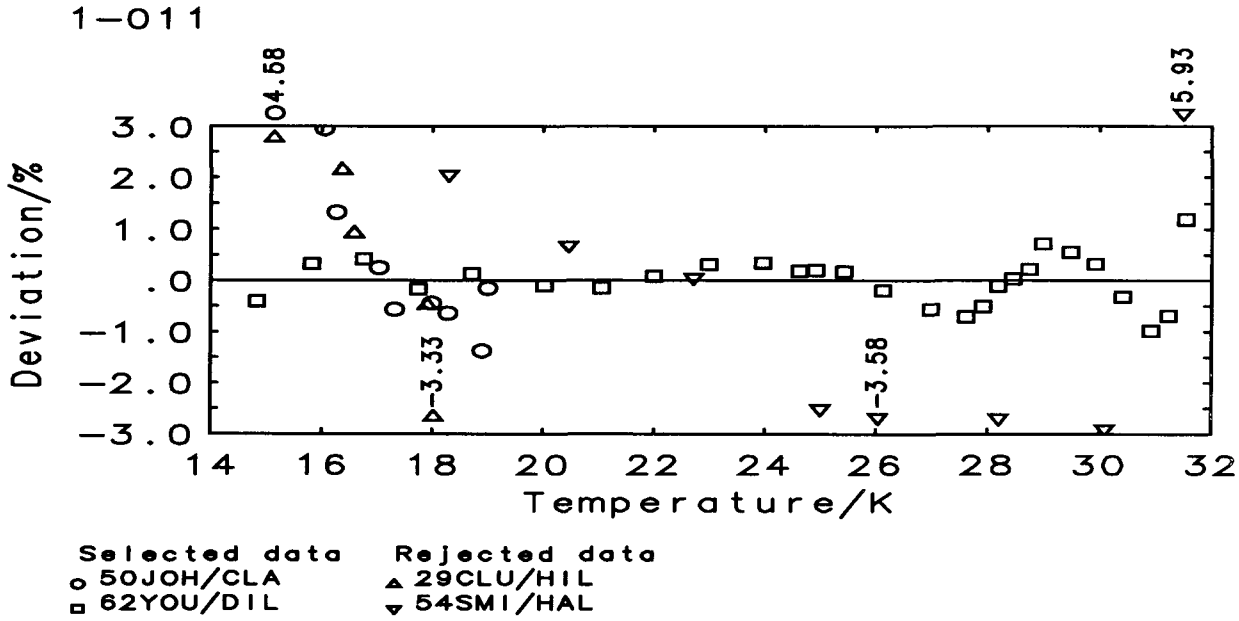
TABLE 1.11.4. Recommended values of heat capacities

Temp. (K)	15	17	19	21	23	25	27
c_p (J K^{-1}g^{-1})	6.904	7.872	8.986	10.22	11.61	13.51	16.32
C_p (J K^{-1}mol^{-1})	13.92	15.87	18.11	20.60	23.41	27.23	32.90
c_{sat} (J K^{-1}g^{-1})	6.904	7.869	8.902	10.01	11.26	12.85	15.06
C_{sat} (J K^{-1}mol^{-1})	13.92	15.86	17.95	20.19	22.69	25.91	30.36
Temp. (K)	29	31					
c_p (J K^{-1}g^{-1})	20.7	31.5					
C_p (J K^{-1}mol^{-1})	41.6	63.5					
c_{sat} (J K^{-1}g^{-1})	18.2	25.3					
C_{sat} (J K^{-1}mol^{-1})	36.8	50.9					

TABLE 1.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	56	39	2.067	4.03–2	0.66	3.88–4	–3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
14.8–31.5	33.00	–9.76684–1	2.18035–1	1.85514–1	1.09376	V



Name: Helium
Formula: He

CAS–RN: 7440–59–7
Group No.: 1–012
Molar Mass: 4.00

TABLE 1.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
35KEE/KEE	1.2–2.3	30	nosp	not specified	C_{sat}	BSIO	35KEE/KEE
51HUL/WIL	0.6–1.6	11S	5.00	not specified	C_{sat}	BSIO	51HUL/WIL
57HIL/LOU	1.8–5.1	46S	1.00	not specified	C_{sat}	BSIO	57HIL/LOU

Name: Helium (isotope of mass 3)
Formula: He

CAS–RN: 14762–55–1
Group No.: 1–013
Molar Mass: 3.02

TABLE 1.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
54OSB/ABR		.0–1.0	eqn	5.00	not specified	C_{sat}	BSIO	54OSB/ABR
54ROB/SYD	N	.5–1.7	14	nosp	not specified	C_{sat}	BSIO	54ROB/SYD
55ROB/SYD	N	.4–2.4	21	2.00	not specified	C_{sat}	BSIO	54ROB/SYD

54ROB/SYD content of He(4) isotope below 0.1 %
55ROB/SYD content of He(4) isotope 0.12 %

Name: Mercury
Formula: Hg

CAS–RN: 7439–97–6
Group No.: 1–014
Molar Mass: 200.59

TABLE 1.14.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
12LUS	N	335.6–363.1	2	nosp	not specified	C_{avg}	DSIO	12LUS
30CAR/STO		236.5–285.1	2	nosp	not specified	C_p	BSIO	30CAR/STO
51DOU/BAL		273.1–733.2	26S	0.10	99.999 anal	C_p	DSTO	50GIN/DOU
53BUS/GIA		239.0–325.9	20	0.10	99.9994 anal	C_p	BSIO	41GIA/MEA
79AMI/LEB		237.9–299.0	14	nosp	99.9998 melpt	C_p	BSAO	79AMI/LEB
88BUN		349.6	1	nosp	not specified	C_p	DDCT	85WAD

TABLE 1.14.2. Correlated heat capacities

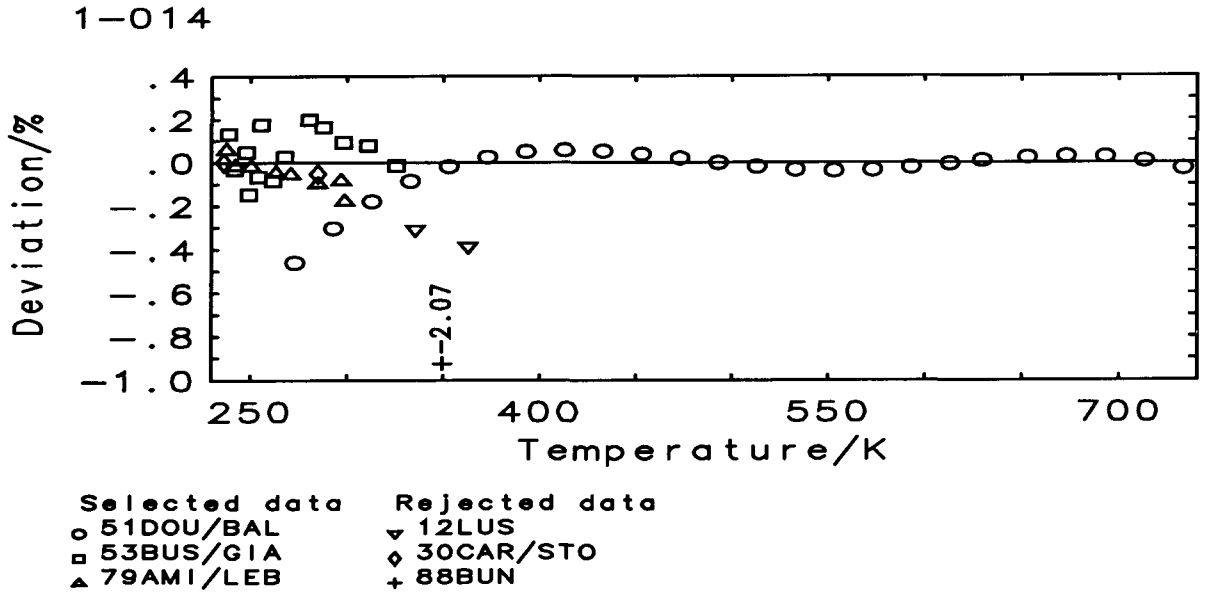
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
51DOU/BAL	273.1–733.2	26	0.10	1.301	4.37–3	0.13	–1.56–3	–3
53BUS/GIA	239.0–325.9	20	0.10	1.148	3.89–3	0.11	2.22–3	10
79AMI/LEB	237.9–299.0	14	0.20#	0.371	2.50–3	0.07	–9.32–4	–6
				Rejected data				
12LUS	(1.16–2, 0.35, –1.16–2, –2)			30CAR/STO	(1.87–3, 0.06, –1.87–3, –1)			
88BUN	(6.73–2, 2.07, –6.73–2, –1)							

TABLE 1.14.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	60	1.146	4.01–3	0.12–1.	55–4	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
237.9–550.0		3.94048	–3.22219–1	5.08152–2	–2.64935–3		II
550.0–733.2		3.18634	8.91258–2	–2.39748–2	1.88337–3		II

TABLE 1.14.4. Recommended values of heat capacities

Temp. (K)	240	260	273.15	280	298.15	300	320
c_p (J K^{-1}g^{-1})	0.142	0.141	0.140	0.140	0.139	0.139	0.139
C_p (J K^{-1}mol^{-1})	28.46	28.27	28.15	28.09	27.95	27.93	27.79
Temp. (K)	340	360	380	400	420	440	460
c_p (J K^{-1}g^{-1})	0.138	0.137	0.137	0.137	0.136	0.136	0.136
C_p (J K^{-1}mol^{-1})	27.67	27.57	27.47	27.40	27.33	27.28	27.24
Temp. (K)	480	500	520	540	560	580	600
c_p (J K^{-1}g^{-1})	0.136	0.135	0.135	0.135	0.135	0.135	0.135
C_p (J K^{-1}mol^{-1})	27.20	27.18	27.16	27.15	27.14	27.14	27.15
Temp. (K)	620	640	660	680	700	720	740
c_p (J K^{-1}g^{-1})	0.135	0.135	0.136	0.136	0.136	0.136	0.137
C_p (J K^{-1}mol^{-1})	27.16	27.18	27.20	27.24	27.28	27.34	27.40



Name: Iodine
Formula: I_2

CAS–RN: 7553–56–2
Group No.: 1–015
Molar Mass: 253.81

TABLE 1.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
37CAR/HAR		389.4–432.7	5	nosp	99.81	anal	C_p	BSIO	30CAR/STO
38FRE/HIL1	N	386.8–433.1	2	1.50	not specified		C_{avg}	DSIO	38FRE/HIL1

38FRE/HIL1 constant value calculated from temperature dependence of enthalpy by the authors

TABLE 1.15.2. *Correlated heat capacities*

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37CAR/HAR	389.4–432.7	5	1.50#	0.800	1.12–1	1.20	2.69–3	–1

TABLE 1.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	5	1.033	1.45–1	1.55	2.69–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
389.4–432.7		1.69634+1	–1.78919				V

TABLE 1.15.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430
c_p ($J K^{-1} g^{-1}$)	0.33	0.32	0.32	0.31	0.30
C_p ($J K^{-1} mol^{-1}$)	83.0	81.5	80.1	78.6	77.1

Name: Indium
Formula: In

CAS–RN: 7440–74–6
Group No.: 1–016
Molar Mass: 114.82

TABLE 1.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33ROT/MEY2		429.1–457.1	2	nosp	not specified		C_p	DSIO	33ROT/MEY2
56SCH/HIL	N	470.5	1	nosp	99.9	anal	C_{avg}	DSIO	56SCH/HIL
63KAZ/ORR		429.3–800.0	5S	nosp	not specified		C_p	not specified	

56SCH/HIL average value in temperature range 433-508 K

TABLE 1.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33ROT/MEY2	429.1–457.1	2	0.70#	0.131	3.24–3	0.09	–2.33–3	–1
63KAZ/ORR	429.3–800.0	5	0.50#	0.083	1.47–3	0.04	4.79–4	1
				Rejected data				
56SCH/HIL	(4.24–2, 1.21, –4.24–2, –1)							

TABLE 1.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.117	2.52–3	0.07	–3.25–4	0
Temp. range K		A_1	A_2				Level of uncertainty
429.1–800.0		3.61555	–1.60987–2				III

TABLE 1.16.4. Recommended values of heat capacities

Temp. (K)	430	480	530	580	630	680	730
c_p ($J K^{-1} g^{-1}$)	0.257	0.256	0.256	0.255	0.254	0.254	0.253
C_p ($J K^{-1} mol^{-1}$)	29.49	29.42	29.35	29.29	29.22	29.15	29.08
Temp. (K)	780	830					
c_p ($J K^{-1} g^{-1}$)	0.253	0.252					
C_p ($J K^{-1} mol^{-1}$)	29.02	28.95					

Name: Potassium
Formula: K

CAS–RN: 7440–09–7
Group No.: 1–017
Molar Mass: 39.10

TABLE 1.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
06BER	343.1–401.6	3	nosp	not specified		C_{avg}	DSTO	06BER
06WIG	340.8–363.1	2	nosp	not specified		C_p	not specified	
13REN	337.0–373.0	eqn	nosp	not specified		C_p	DSIO	13REN
39CAR/STE	336.9–609.5	31	nosp	99.92	melpt	C_p	BSIO	30CAR/STO
52DOU/BAL	348.1-1073.2	9S	0.30	99.85	melpt	C_{sat}	DSTO	50GIN/DOU

TABLE 1.17.2. Correlated heat capacities

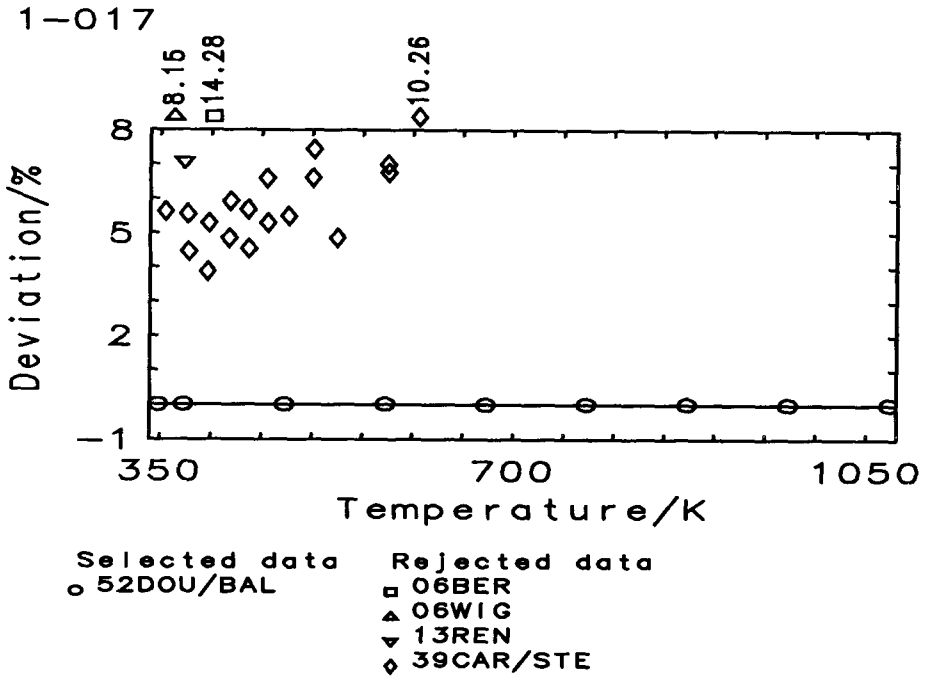
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
52DOU/BAL	348.1	9	0.30	0.016	1.73–4	0.00	–2.65–7	0
				Rejected data				
06BER	(5.43–1, 12.42, 5.34–1, 2)			06WIG	(3.40–1, 8.15, 3.40–1, 1)			
13REN	(2.91–1, 7.07, 2.91–1, 1)			39CAR/STE	(2.53–1, 6.35, 2.43–1, 23)			

TABLE 1.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	47	9	0.019	2.11–4	0.01	–2.65–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
348.1–1073.2		4.47054	–2.29700–1	1.47774–2			II

TABLE 1.17.4. Recommended values of heat capacities

Temp. (K)	350	400	450	500	550	600	650
c_{sat} ($J\,K^{-1}g^{-1}$)	0.818	0.806	0.795	0.785	0.777	0.771	0.766
C_{sat} ($J\,K^{-1}mol^{-1}$)	31.99	31.50	31.06	30.69	30.38	30.13	29.95
Temp. (K)	700	750	800	850	900	950	1000
c_{sat} ($J\,K^{-1}g^{-1}$)	0.763	0.761	0.761	0.763	0.766	0.770	0.776
C_{sat} ($J\,K^{-1}mol^{-1}$)	29.82	29.76	29.76	29.81	29.93	30.12	30.36
Temp. (K)	1050						
c_{sat} ($J\,K^{-1}g^{-1}$)	0.784						
C_{sat} ($J\,K^{-1}mol^{-1}$)	30.66						



Name: Krypton
Formula: Kr

CAS–RN: 7439–90–9
Group No.: 1–018
Molar Mass: 83.80

TABLE 1.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
36CLU	118.3–120.5	4	nosp	not specified	C_{sat}	BSIO	36CLU/GOL
38CLU/KRU	117.1–123.1	6	nosp	not specified	C_{sat}	BSIO	36CLU/GOL
61BEA/CHI	116.5–118.4	5	0.50	99.9995 melpt	C_p	BSAO	61FLU/LEA

TABLE 1.18.2. Correlated heat capacities

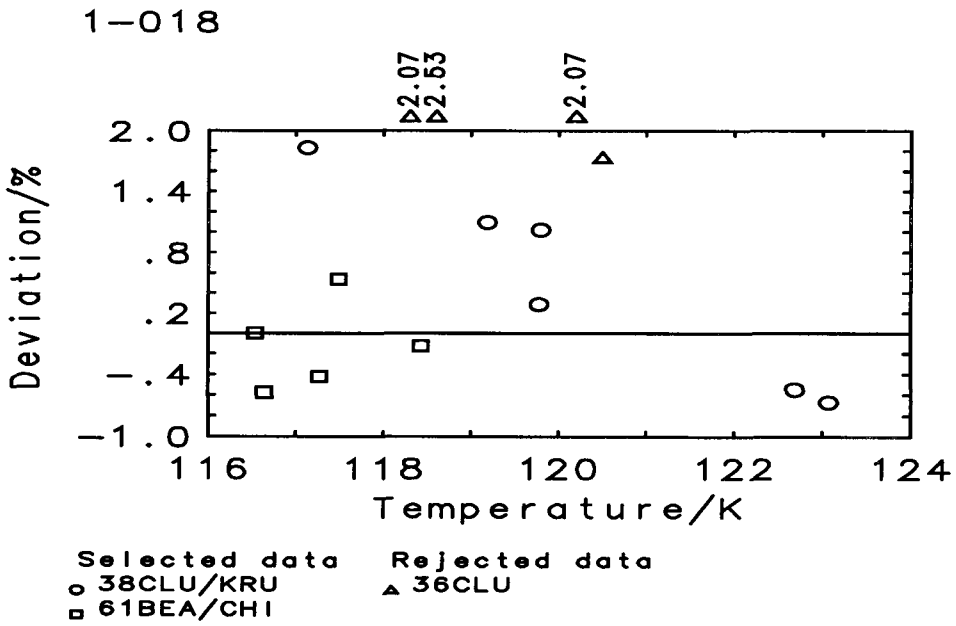
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
38CLU/KRU	117.1–123.1	6	1.00#	1.034	5.54–2	1.03	2.67–2	2
61BEA/CHI	116.5–118.4	5	0.50	0.817	2.14–2	0.41	–7.49–3	–3
				Rejected data				
36CLU	(1.15–1, 2.12, 1.14–1, 4)							

TABLE 1.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	11	1.041	4.79–2	0.90	1.11–2	–1
C_{sat}	15	11	1.045	4.80–2	0.90	1.12–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
116.5–123.1		1.48874	3.20386				IV
116.5–123.1		1.59216	3.10704				IV

TABLE 1.18.4. Recommended values of heat capacities

Temp. (K)	117	119	121	123
c_p (J K^{-1}g^{-1})	0.520	0.526	0.532	0.539
C_p (J K^{-1}mol^{-1})	43.55	44.08	44.61	45.14
c_{sat} (J K^{-1}g^{-1})	0.519	0.525	0.531	0.537
C_{sat} (J K^{-1}mol^{-1})	43.46	43.98	44.50	45.01



Name: Lithium
Formula: Li

CAS-RN: 7439-93-2
Group No.: 1-019
Molar Mass: 6.94

TABLE 1.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
50YAG/UNT		473.1-773.2	4	10.00	99.7	chrom	C_p	BDHO	50YAG/UNT
51BAT/SMI	N	673.0-1273.0	2	nosp	not specified		C_p	not specified	
52RED/LON	N	523.0-1373.0	eqn	5.00	99.9	anal	C_p	DSTO	52RED/LON
55DOU/EPS		453.7-1200.0	24S	0.30	99.989	melpt	C_p	DSTO	50GIN/DOU

51BAT/SMI authors give a constant C_p over the entire temperature range
52RED/LON calculated from temperature dependence of enthalpy by the authors

TABLE 1.19.2. Correlated heat capacities

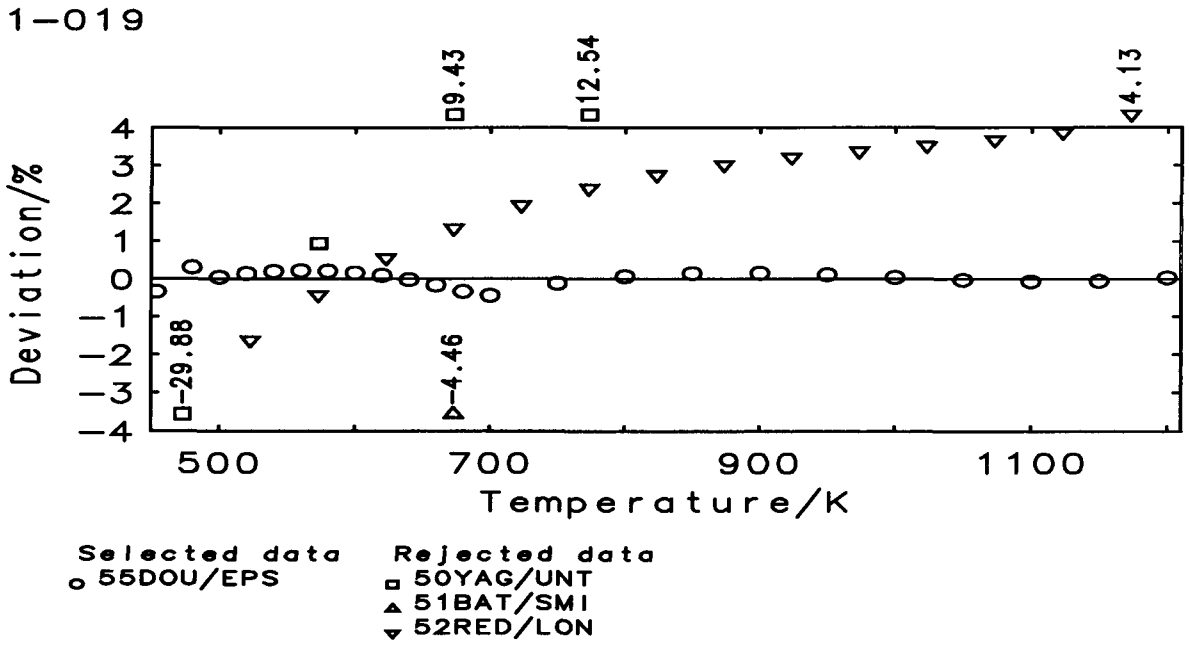
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
55DOU/EPS	453.7-1200.0	24	0.30	0.648	6.92-3	0.19	2.61-5	4
				Rejected data				
50YAG/UNT	(5.22-1, 16.88, 1.48-2, 2)			51BAT/SMI	(1.50-1, 4.47, -1.50-1, -1)			
52RED/LON	(1.01-1, 2.81, 8.12-2, 10)							

TABLE 1.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	48	24	0.710	7.59-3	0.21	2.61-5	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
453.7-1200.0		4.68445	-3.64142-1	3.63908-2	-1.21532-3		III

TABLE 1.19.4. Recommended values of heat capacities

Temp. (K)	460	510	560	610	660	710	760
c_p (J K^{-1}g^{-1})	4.386	4.328	4.280	4.242	4.213	4.191	4.175
C_p (J K^{-1}mol^{-1})	30.44	30.04	29.71	29.45	29.24	29.09	28.98
Temp. (K)	810	860	910	960	1010	1060	1110
c_p (J K^{-1}g^{-1})	4.165	4.158	4.155	4.153	4.153	4.152	4.150
C_p (J K^{-1}mol^{-1})	28.91	28.86	28.84	28.83	28.82	28.82	28.80
Temp. (K)	1160	1210					
c_p (J K^{-1}g^{-1})	4.145	4.137					
C_p (J K^{-1}mol^{-1})	28.77	28.71					



Name: Nitrogen
Formula: N_2

CAS–RN: 7727–37–9
Group No.: 1–020
Molar Mass: 28.01

TABLE 1.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type Reference
16EUC	64.6–72.7	5	nosp	not specified	C_{sat}	BSIO 16EUC
29CLU1	66.9–73.5	5	0.70	not specified	C_p	BSIO 29CLU1
30WIE/BRE	79.2–117.0	14	2.00	not specified	C_{sat}	BSIO 30WIE/HUB
33GIA/CLA	65.0–77.7	7	0.80	99.997 melpt	C_p	BSIO 28GIA/WIE1
59CLU/SPE	65.9–68.2	4	nosp	not specified	C_p	not specified
81WEB	78.5–124.8	43	0.60	99.99 estim	C_{sat}	BSAO 61GOO
91MAG	64.8–120.7	102	0.50	99.9998 anal	C_{sat}	BSAO 61GOO

TABLE 1.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33GIA/CLA	65.0–77.7	7	0.80	0.323	1.75–2	0.26	4.24–3	1
81WEB	78.5–124.8	43	0.60	1.887	2.39–1	1.13	1.06–3	1
91MAG	64.8–120.7	102	0.50	0.471	2.23–2	0.24	1.81–3	18
				Rejected data				
16EUC	(6.91–2, 1.03, –6.32–2, –4)			29CLU1	(8.44–2, 1.23, 8.23–2, 5)			
30WIE/BRE	(2.22–1, 2.14, –7.46–2, –2)			59CLU/SPE	(6.00–2, 0.88, 4.84–2, 3)			

TABLE 1.20.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	180	152	1.100	1.31–1	0.65	1.71–3	20
C_{sat}	180	152	1.279	1.31–1	0.76	2.06–3	15
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
64.8–105.0		–1.14490+1	7.04695+1	–9.20497+1	4.08251+1		III
105.0–118.0		–7.74321+2	2.25011+3	–2.16789+3	6.99823+2		IV
118.0–124.8		–4.28969+4	1.09341+5	–9.29231+4	2.63369+4		VI
64.8–105.0		–5.70805	4.80807+1	–6.28551+1	2.80389+1		III
105.0–118.0		–4.62439+2	1.35303+3	–1.30566+3	4.22581+2		IV
118.0–124.8		–3.73354+4	9.50979+4	–8.07505+4	2.28646+4		VI

TABLE 1.20.4. Recommended values of heat capacities

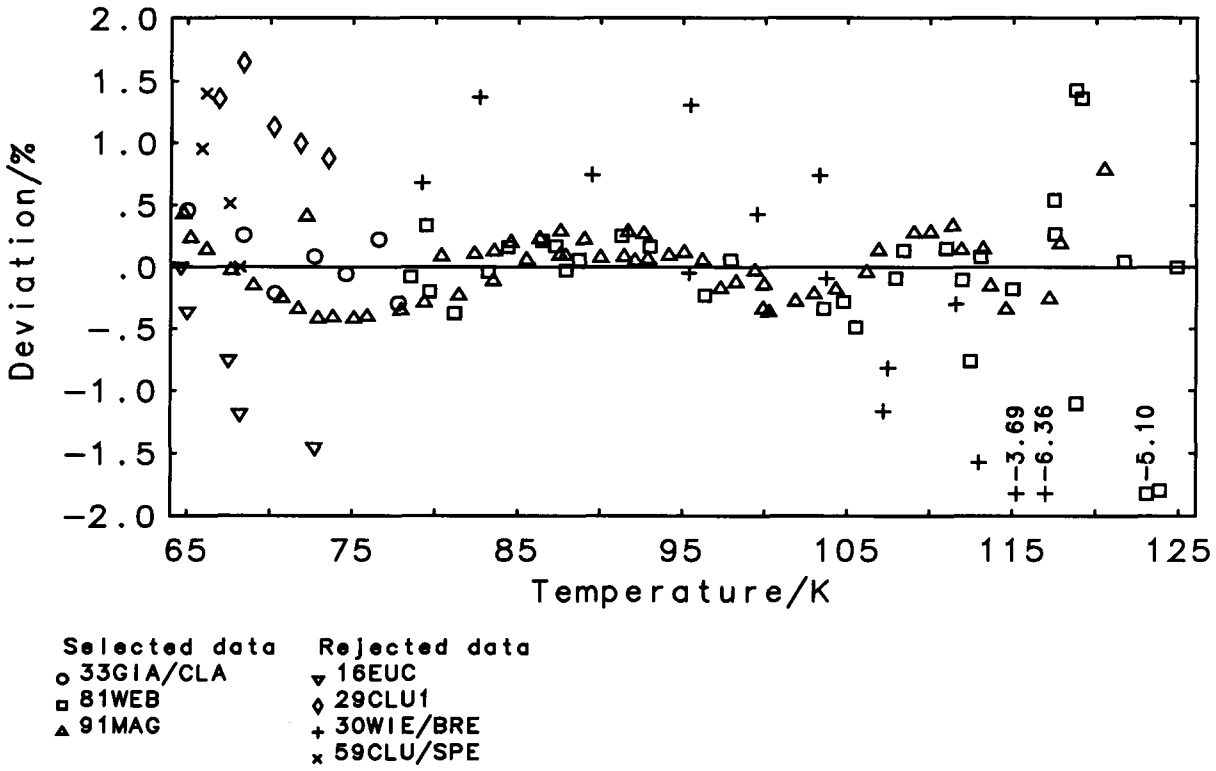
Temp. (K)	65	70	75	80	85	90	95
c_p ($J\,K^{-1}g^{-1}$)	1.982	2.012	2.033	2.053	2.082	2.130	2.204
C_p ($J\,K^{-1}mol^{-1}$)	55.51	56.36	56.94	57.51	58.33	59.66	61.73
c_{sat} ($J\,K^{-1}g^{-1}$)	1.985	2.008	2.026	2.044	2.068	2.105	2.161
C_{sat} ($J\,K^{-1}mol^{-1}$)	55.61	56.26	56.75	57.25	57.93	58.97	60.54
Temp. (K)	100	105	110	115	120	125	
c_p ($J\,K^{-1}g^{-1}$)	2.314	2.469	2.703	3.147	4.02	7.90	
C_p ($J\,K^{-1}mol^{-1}$)	64.82	69.17	75.73	88.17	113	221	
c_{sat} ($J\,K^{-1}g^{-1}$)	2.243	2.356	2.521	2.819	3.40	6.47	
C_{sat} ($J\,K^{-1}mol^{-1}$)	62.83	66.00	70.63	78.96	95.1	181	

TABLE 1.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	180	152	1.724	1.17–1	0.95	–1.39–3	15

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
64.8–124.8	126.20	–2.64196	1.38507–1	1.50586	2.58845+1	–5.31133+1	2.86788+1	V

1-020



Name: Sodium
Formula: Na

CAS-RN: 7440-23-5
Group No.: 1-021
Molar Mass: 22.99

TABLE 1.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
06BER	N	401.6	1	nosp	not specified	C_{avg}	DSTO	06BER
13REN		371.1	1	nosp	not specified	C_p	DSIO	13REN
14GRI		374.0–411.6	5	nosp	not specified	C_p	BSIO	14GRI
50GIN/DOU		371.0-1173.0	10S	0.40	99.9984 melpt	C_{sat}	DSTO	50GIN/DOU
56SCH/HIL	N	483.0	1	nosp	not specified	C_{avg}	DSIO	56SCH/HIL

06BER average value in temperature range 373–430 K
56SCH/HIL average value in temperature range 463–503 K

TABLE 1.21.2. Correlated heat capacities

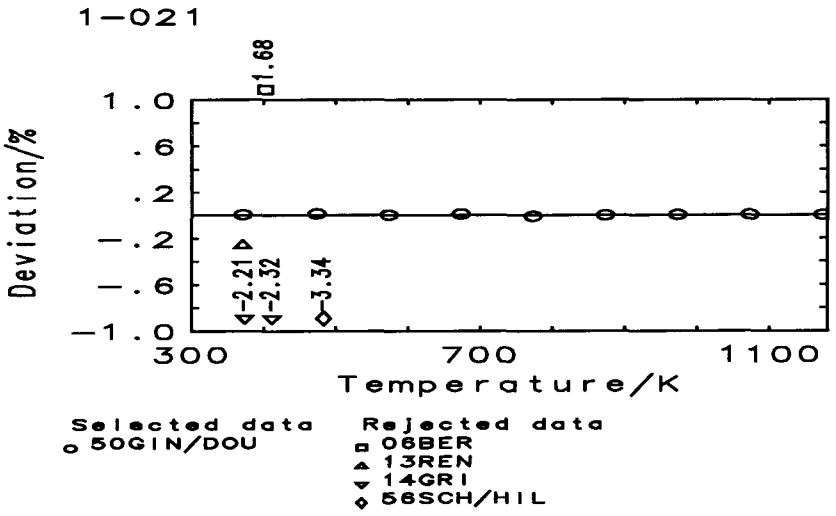
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50GIN/DOU	371.0–1173.0	10	0.40	0.017	2.53–4	0.01	1.19–7	–1
				Rejected data				
06BER	(6.48–2, 1.68, 6.48–2, 1)			13REN	(1.00–2, 0.26, –1.00–2, –1)			
14GRI	(8.24–2, 2.21, –8.24–2, –5)			56SCH/HIL	(1.19–1, 3.34, –1.19–1, –1)			

TABLE 1.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	10	0.021	3.02–4	0.01	1.19–7	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
371.0–1173.0		4.50689	–2.30446–1	1.27872–2			III

TABLE 1.21.4. Recommended values of heat capacities

Temp. (K)	380	430	480	530	580	630	680
c_{sat} (J K^{-1}g^{-1})	1.380	1.357	1.336	1.318	1.302	1.288	1.277
C_{sat} (J K^{-1}mol^{-1})	31.73	31.20	30.73	30.30	29.94	29.62	29.36
Temp. (K)	730	780	830	880	930	980	1030
c_{sat} (J K^{-1}g^{-1})	1.268	1.261	1.257	1.255	1.255	1.257	1.262
C_{sat} (J K^{-1}mol^{-1})	29.15	29.00	28.89	28.84	28.85	28.91	29.02
Temp. (K)	1080	1130	1180				
c_{sat} (J K^{-1}g^{-1})	1.269	1.279	1.290				
C_{sat} (J K^{-1}mol^{-1})	29.18	29.40	29.67				



Name: Neon
Formula: Ne

CAS–RN: 7440–01–9
Group No.: 1–022
Molar Mass: 20.18

TABLE 1.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
29CLU2	27.8–41.8	6	1.50	not specified		C_{sat}	BSIO	29CLU1
36CLU	25.7–26.8	4	nosp	not specified		C_{sat}	BSIO	36CLU/GOL

TABLE 1.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
29CLU2	37.9–41.8	4	1.50	1.135	1.12–1	1.70	5.24–3	2
36CLU	25.7–26.8	4	1.50#	0.161	1.06–2	0.24	–7.46–4	0

TABLE 1.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	8	1.147	1.12–1	1.72	2.25–3	2
C_{sat}	10	8	1.370	1.28–1	2.06	2.52–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
25.7–41.8	–6.26990+1	6.65671+2	–2.20106+3	2.43611+3	V
25.7–41.8	–2.64403+1	2.98063+2	–9.68020+2	1.06744+3	V

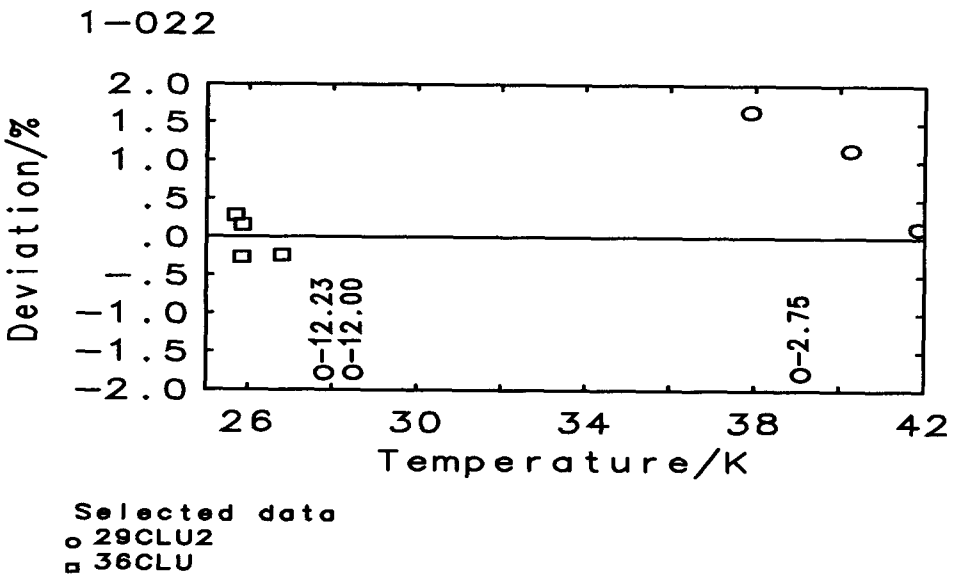
TABLE 1.22.4. Recommended values of heat capacities

Temp. (K)	25	30	35	40
c_p ($J\,K^{-1}g^{-1}$)	1.74	1.93	2.10	3.01
C_p ($J\,K^{-1}mol^{-1}$)	35.1	38.9	42.4	60.8
c_{sat} ($J\,K^{-1}g^{-1}$)	1.75	1.93	2.09	2.56
C_{sat} ($J\,K^{-1}mol^{-1}$)	35.4	38.9	42.1	51.7

TABLE 1.22.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	8	1.331	1.42–1	2.00	6.09–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
25.7–41.8	44.40	–7.46473–1	1.94151–1	2.83415	7.17511–1	V



Name: Oxygen
Formula: O_2

CAS–RN: 7782–44–7
Group No.: 1–023
Molar Mass: 32.00

TABLE 1.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
16EUC		57.4–73.0	7	nosp	not specified		C_{sat}	BSIO	16EUC
29CLU1		56.6–72.8	13	0.70	not specified		C_p	BSIO	29CLU1
29GIA/JOH	N	57.0–90.3	24	nosp	not specified		C_p	BSIO	28GIA/WIE1
69GOO/WEB		56.4–152.4	88	nosp	99.99	anal	C_{sat}	BSAO	61GOO

29GIA/JOH high sample purity

TABLE 1.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
29GIA/JOH	57.0–90.3	24	0.50#	0.568	1.84–2	0.28	1.15–2	11
69GOO/WEB	56.4–152.4	88	0.30#	1.166	3.20–2	0.35	–7.98–4	–6
				Rejected data				
16EUC	(3.42–2, 0.54, 3.68–3, 1)			29CLU1	(9.37–2, 1.48, –5.18–2, –6)			

TABLE 1.23.3. Parameters of cubic spline polynomials

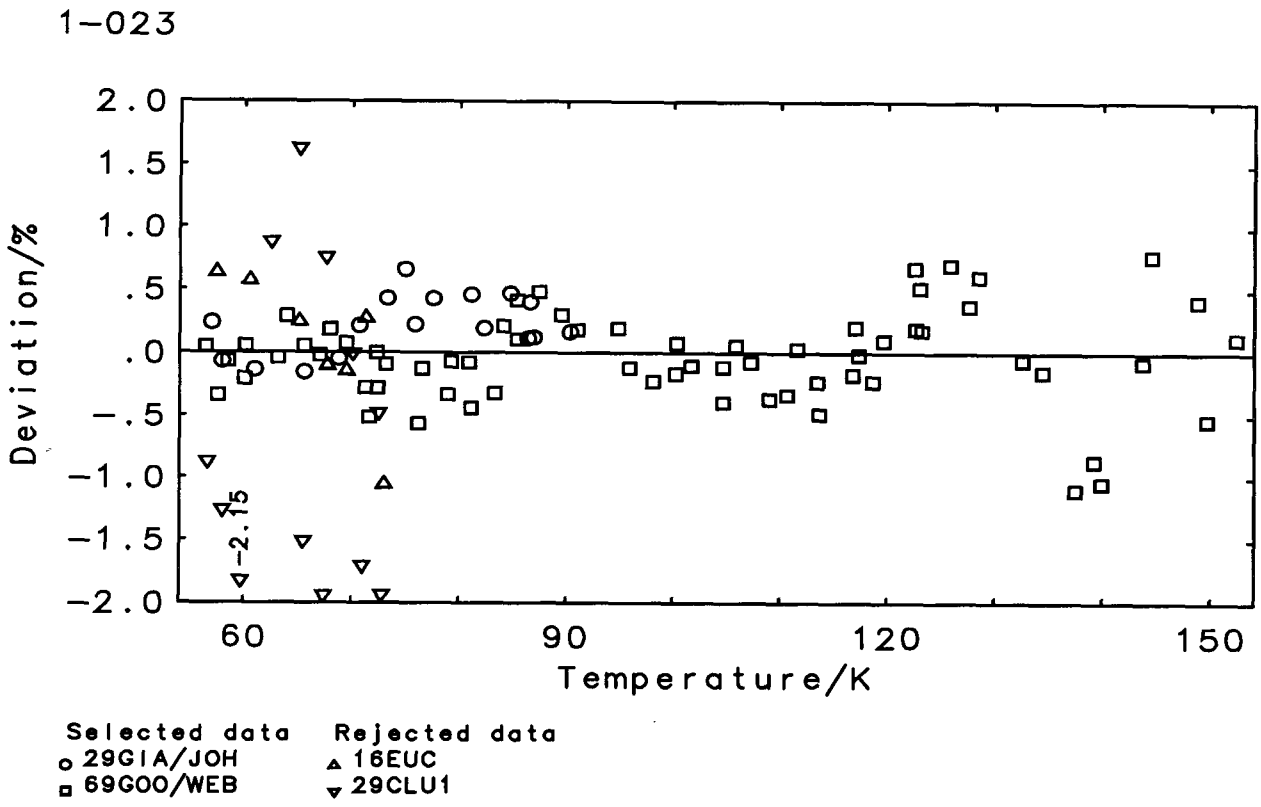
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	132	112	1.102	3.05–2	0.35	1.84–3	5
C_{sat}	132	112	1.045	2.94–2	0.33	1.79–3	5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
56.4–90.0		6.11269	1.89527	–3.84283	2.49240		II
90.0–120.0		1.01011	1.89039+1	–2.27413+1	9.49182		III
120.0–144.0		–2.54928+2	6.58750+2	–5.55946+2	1.57604+2		III
144.0–152.4		–3.67917+4	7.67771+4	–5.34159+4	1.23937+4		V
56.4–90.0		6.40740	5.63030–1	–1.84056	1.49122		II
90.0–120.0		2.39592	1.39347+1	–1.66979+1	6.99395		III
120.0–144.0		–1.60486+2	4.21139+2	–3.56035+2	1.01254+2		III
144.0–152.4		–3.17377+4	6.62069+4	–4.60406+4	1.06764+4		V

TABLE 1.23.4. Recommended values of heat capacities

Temp. (K)	60	70	80	90	100	110	120
c_p (J K^{-1}g^{-1})	1.664	1.666	1.675	1.695	1.732	1.798	1.910
C_p (J K^{-1}mol^{-1})	53.25	53.31	53.59	54.23	55.41	57.55	61.10
c_{sat} (J K^{-1}g^{-1})	1.664	1.666	1.674	1.692	1.722	1.774	1.860
C_{sat} (J K^{-1}mol^{-1})	53.25	53.31	53.57	54.13	55.10	56.78	59.52
Temp. (K)	130	140	150				
c_p (J K^{-1}g^{-1})	2.119	2.633	4.38				
C_p (J K^{-1}mol^{-1})	67.80	84.25	140				
c_{sat} (J K^{-1}g^{-1})	2.014	2.370	3.68				
C_{sat} (J K^{-1}mol^{-1})	64.45	75.84	118				

TABLE 1.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	132	112	2.314	9.11–2	0.72	–4.45–3	–15
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
56.4–152.4	154.58	–2.28256	1.49832–1	4.54619	8.83694	–2.50571+1	1.49298+1	V



Name: Ozone
Formula: O_3

CAS-RN: 10028-15-6
Group No.: 1-024
Molar Mass: 48.00

TABLE 1.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
58BRA/WAT	N	96.5–122.9	6	nosp	not specified	C_p	BDHT	58BRA/WAT

58BRA/WAT error increasing from 2 to 8 % between lower and upper temperature limits

TABLE 1.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	1.191	6.70–1	5.95	5.28–2	2
Temp. range K		A_1	A_2				Level of uncertainty
96.6–122.9		8.51603	2.15555				V

TABLE 1.24.4. Recommended values of heat capacities

Temp. (K)	100	110	120
c_p (J K^{-1}g^{-1})	1.85	1.89	1.92
C_p (J K^{-1}mol^{-1})	88.7	90.5	92.3

Name: Phosphorus mol.(P_4)
Formula: P_4

CAS-RN: 12185-10-3
Group No.: 1-025
Molar Mass: 123.90

TABLE 1.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
42YOU/HIL	N	298.0–370.0	eqn	nosp	not specified		C_p	DSIO	42YOU/HIL

42YOU/HIL low temperature limit is below n.m.t.; undercooled liquid

TABLE 1.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.000	7.21-7	0.00	-3.82-7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
298.0–370.0	1.21480+1	6.00450-1	-1.97613-1	IV

TABLE 1.25.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	0.817	0.813	0.808	0.804	0.799	0.794	0.788
C_p (J K^{-1}mol^{-1})	101.2	100.7	100.2	99.59	98.99	98.35	97.68

Temp. (K)	370
c_p (J K^{-1}g^{-1})	0.783
C_p (J K^{-1}mol^{-1})	96.98

Name: Rubidium
Formula: Rb

CAS-RN: 7440-17-7
Group No.: 1-026
Molar Mass: 85.47

TABLE 1.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
13REN	312.0–373.0	eqn	nosp	not specified		C_p	DSIO	13REN

TABLE 1.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.000	1.51–7	0.00	6.81–8	0
Temp. range K		A_1	A_2				Level of uncertainty
312.0–373.2		4.26656	–1.11823–1				VI

TABLE 1.26.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	0.38	0.38	0.38	0.38	0.38	0.37
C_p ($J K^{-1} mol^{-1}$)	32.5	32.4	32.3	32.2	32.1	32.0

Name: Sulfur
Formula: S

CAS-RN: 7704-34-9
Group No.: 1-027
Molar Mass: 121.75

TABLE 1.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
54BRA/MOE	393.1–693.2	31S	0.50	not specified		C_p	BSAO	54BRA/MOE
59WES1	388.4–717.8	43S	0.20	99.999	melpt	C_p	BSAO	68WES/WES
67PAC	418.1	1	nosp	not specified		C_p	BDHT	79DU/COM
73KOM/MIL	393.1–598.2	43S	nosp	99.999	melpt	C_p	BDHO	73KOM/MIL
75MON	405.8–433.3	14	nosp	99.999	melpt	C_{sat}	BSAO	75MON

TABLE 1.27.2a. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KOM/MIL	393.1–432.1	9	0.50#	1.189	2.33–2	0.59	1.34–4	1
				Rejected data				
54BRA/MOE	(9.25–2, 2.38, 8.72–2, 4)			59WES1	(8.37–1, 15.59, 6.49–1, 8)			
67PAC	(5.84–1, 13.41, 5.84–1, 1)			75MON	(1.08, 17.93, 7.59–1, 11)			

TABLE 1.27.2b. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KOM/MIL	438.1–598.2	33	0.50#	1.089	2.87–2	0.54	3.93–4	1
				Rejected data				
54BRA/MOE	(1.59–1, 3.50, 2.96–2, 0)			59WES1	(2.16–1, 4.65, 1.04–1, 4)			

TABLE 1.27.3a. Parameters of regression polynomial

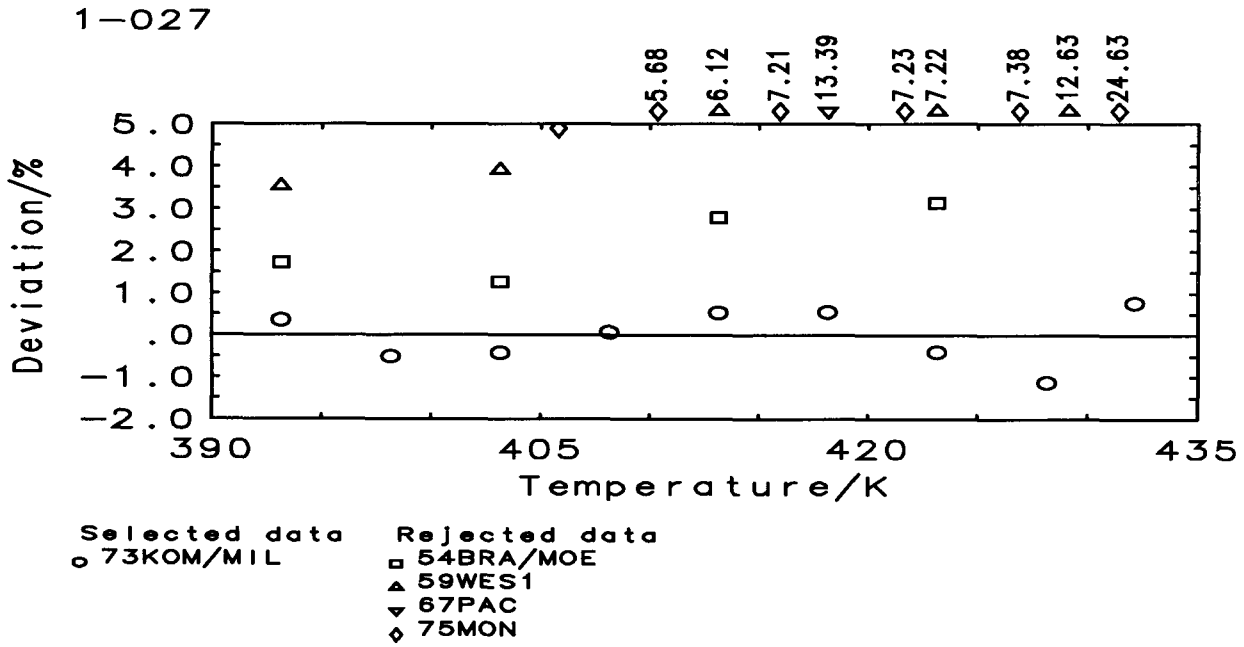
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C	132	9	1.596	3.13–2	0.80	1.34–4	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
393.1–432.1		−1.85689+3	1.37277+3	−3.37560+2	2.76644+1		IV

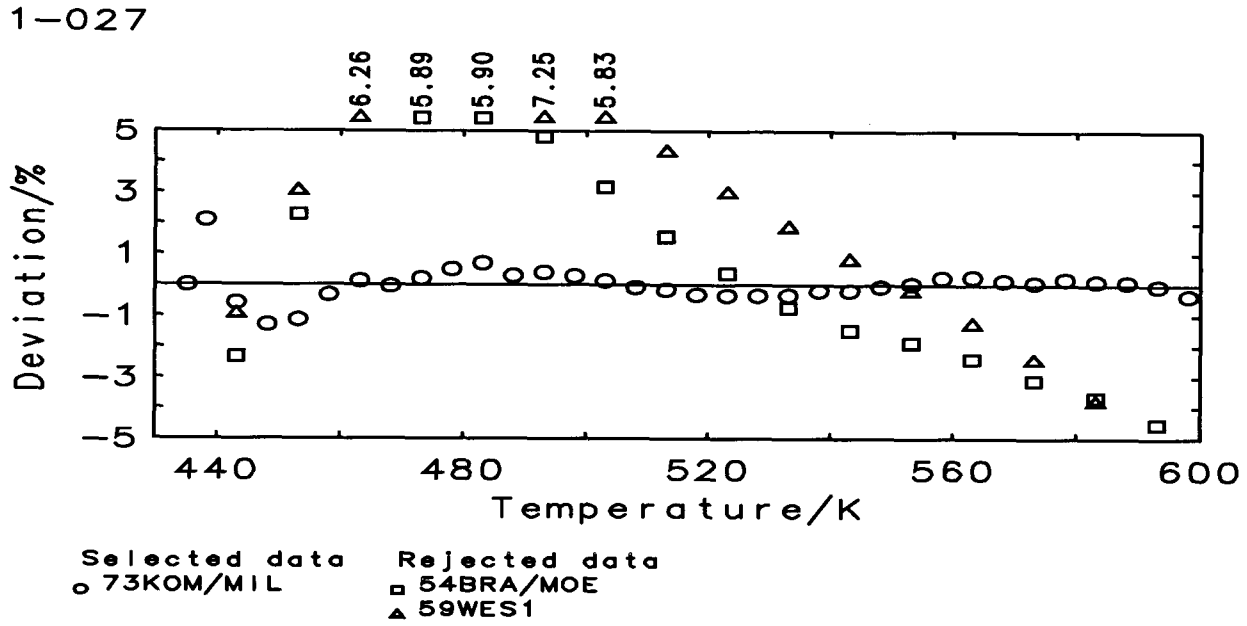
TABLE 1.27.3b. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	132	33	1.182	3.12–2	0.59 3.	93–4	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
438.1–510.0		5.90051+2	−3.46559+2	6.83281+1	−4.48944		IV
510.0–598.2		−6.70282+1	3.99583+1	−7.45952	4.64001−1		IV

TABLE 1.27.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430		
c_p (J K^{-1}g^{-1})	0.948	0.975	0.972	0.984	1.052		
C_p (J K^{-1}mol^{-1})	30.40	31.25	31.17	31.54	33.74		
Temp. (K)	440	450	460	470	480	490	500
c_p (J K^{-1}g^{-1})	1.451	1.317	1.224	1.163	1.129	1.113	1.110
C_p (J K^{-1}mol^{-1})	46.53	42.25	39.24	37.30	36.19	35.70	35.59
Temp. (K)	510	520	530	540	550	560	570
c_p (J K^{-1}g^{-1})	1.112	1.113	1.113	1.112	1.112	1.113	1.116
C_p (J K^{-1}mol^{-1})	35.65	35.68	35.69	35.67	35.67	35.70	35.79
Temp. (K)	580	590	600				
c_p (J K^{-1}g^{-1})	1.121	1.129	1.142				
C_p (J K^{-1}mol^{-1})	35.95	36.22	36.61				





Name: Selenium
Formula: Se

CAS-RN: 7782-49-2
Group No.: 1-028
Molar Mass: 78.96

TABLE 1.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
26MON		490.1	1	nosp	not specified	C_p	DSIO	26MON
64GAT/HEI	N	503.1–533.2	4S	nosp	not specified	C_p	DSIO	63GAT/KRE
73GRO		502.9–994.1	48	nosp	99.9992 melpt	C_p	BSAO	67GRO
90JIN/WUN		523.2–548.2	2	nosp	99.999 anal	C_p	BDHT	90JIN/WUN

64GAT/HEI high purity of substance with traces of Al and Cu (0.0001 %)

TABLE 1.28.2. Correlated heat capacities

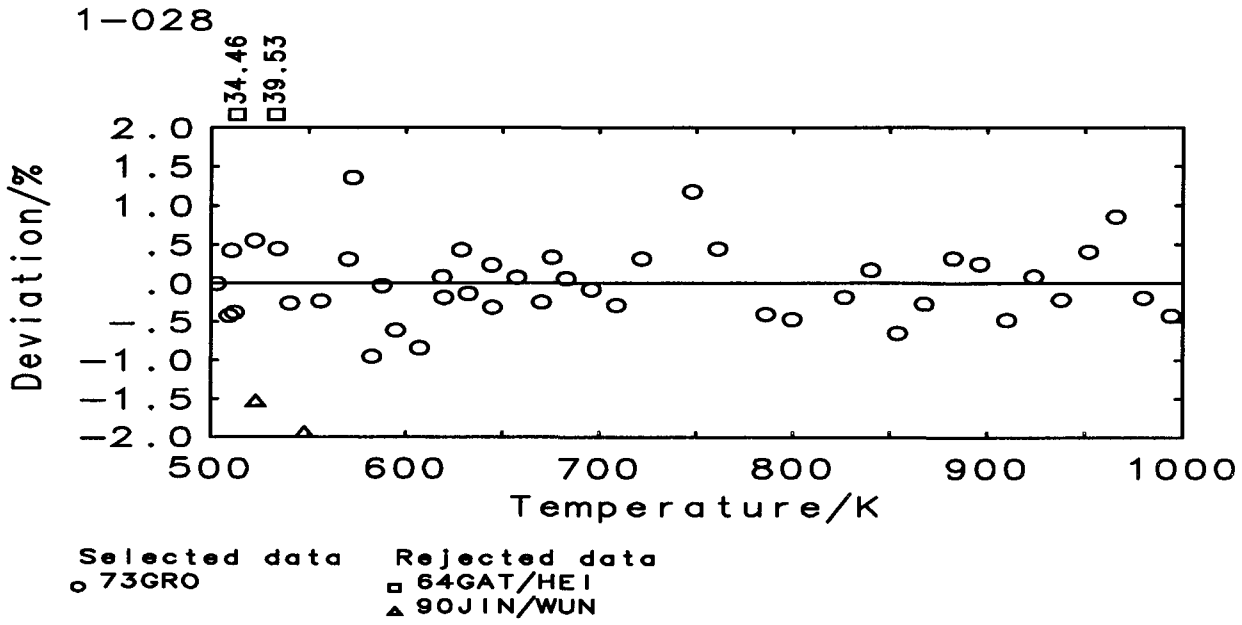
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73GRO	509.3–994.1	47	0.50#	0.921	1.91–2	0.46	1.76–4	–3
				Rejected data				
64GAT/HEI	(2.60, 37.68, 2.59, 3)		90JIN/WUN	(7.38–2, 1.77, –7.34–2, –2)				

TABLE 1.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	55	47	0.963	2.00–2	0.48	1.76–4	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
509.3–994.1		5.18010	–4.35497–2	–4.66559–2	4.21206–3		III

TABLE 1.28.4. Recommended values of heat capacities

Temp. (K)	510	560	610	660	710	760	810
c_p ($J K^{-1} g^{-1}$)	0.453	0.444	0.435	0.429	0.424	0.422	0.422
C_p ($J K^{-1} mol^{-1}$)	35.78	35.03	34.38	33.85	33.48	33.29	33.30
Temp. (K)	860	910	960				
c_p ($J K^{-1} g^{-1}$)	0.425	0.431	0.441				
C_p ($J K^{-1} mol^{-1}$)	33.54	34.04	34.83				



HEAT CAPACITY OF LIQUIDS

Name: Tin
Formula: Sn

CAS-RN: 7440-31-5
Group No.: 1-029
Molar Mass: 118.71

TABLE 1.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AWB/GRI	N	503.1–573.2	2	nosp	99.98	anal	C_p	DSIO	26AWB/GRI
26UMI		523.2–873.2	8S	nosp	99.989	anal	C_{avg}	not specified	
47BAR		523.2–623.2	3S	1.00	99.84	anal	C_p	BDHO	40TUR/BAR
63KAZ/ORR		505.0–800.0	5S	nosp	not specified		C_p	not specified	
69FEB/HER	N	1222.0–1745.0	2	0.70	not specified		C_p	DSAO	62LEV

26AWB/GRI constant value calculated from temperature dependence of enthalpy by the authors
69FEB/HER constant value calculated from temperature dependence of enthalpy by the authors

TABLE 1.29.2. Correlated heat capacities

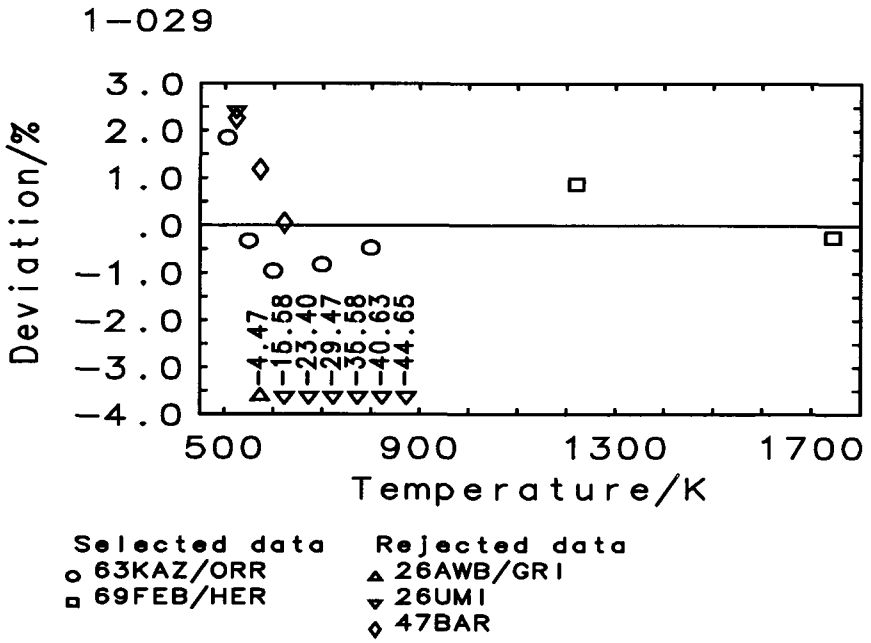
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
63KAZ/ORR	505.0–800.0	5	0.80#	1.295	3.66–2	1.04	–4.74–3	–3
69FEB/HER	1222.0–1745.0	2	0.70	0.916	2.23–2	0.64	1.08–2	0
				Rejected data				
26AWB/GRI	(1.49–1, 4.47, –1.49–1, –1)			26UMI	(7.34–1, 28.79, –6.31–1, –6)			
47BAR	(5.25–2, 1.47, 4.15–2, 3)							

TABLE 1.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	20	7	1.586	4.38–2	1.24	–2.99–4	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
505.0–1745.0		3.63461	–3.20295–2	1.33065–3			V

TABLE 1.29.4. Recommended values of heat capacities

Temp. (K)	510	610	710	810	910	1010	1110
c_p ($J K^{-1} g^{-1}$)	0.25	0.24	0.24	0.24	0.24	0.24	0.24
C_p ($J K^{-1} mol^{-1}$)	29.1	29.0	28.9	28.8	28.7	28.7	28.6
Temp. (K)	1210	1310	1410	1510	1610	1710	
c_p ($J K^{-1} g^{-1}$)	0.24	0.24	0.24	0.24	0.24	0.24	
C_p ($J K^{-1} mol^{-1}$)	28.6	28.6	28.7	28.7	28.8	28.9	



Name: Xenon
Formula: Xe

CAS–RN: 7440–63–3
Group No.: 1–030
Molar Mass: 131.29

TABLE 1.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38CLU/RIC	163.2–165.9	7	nosp	not specified		C_{sat}	BSIO	36CLU/GOL

TABLE 1.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.710	2.67–2	0.50	1.90–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
163.2 –165.9		5.18191	1.17549–1				IV

TABLE 1.30.4. Recommended values of heat capacities

Temp. (K)	163	164	165	166
c_{sat} (J K^{-1}g^{-1})	0.340	0.340	0.340	0.341
C_{sat} (J K^{-1}mol^{-1})	44.68	44.69	44.70	44.71

02. Inorganic Compounds

The family of inorganic compounds contains 103 compounds, 12 of which were measured at one temperature only.

Similar to the family containing elements, the family of inorganic compounds has a significantly different character from most of the organic compounds in this compilation. In general, the only unifying feature may be that their melting temperature is below 573 K. Measurements were performed in a large number of diverse laboratories. Special attention is paid to some industrially important compounds.

The largest number of measurements, 22, were carried out at UCB by the group of Professor W.F. Giauque (1949 Nobel Laureate in chemistry) over a period of 30 years. All measurements from this laboratory were carried out in an isoperibol calorimeter and were included in the correlation with a claimed uncertainty of 0.3 % (with the exception of nitric oxide, NO, where the claimed error was 1 %). The group of compounds measured at UCB is very diverse and some compounds were measured only at this laboratory. Hydroiodic acid and hydrogen sulfide were investigated in other laboratories, but only the data from UCB (29GIA/WIE, 36GIA/BLU) have been considered in the final correlation. For sulfuric acid, ammonia, and nitric oxide, NO, the data measured at UCB (52RUB/GIA, 37OVE/GIA, 29JOH/GIA) have been merged with less accurate data from other laboratories (24EUC/KAR, 26DAN/JEN, 32SOC, 57KER, 71POP/MAN) in order to extend the temperature interval of the recommended data. Reliable data from UCB for hydrobromic acid (28GIA/WIE2), hydrochloric acid (28GIA/WIE1) and nitrous oxide, N_2O, (35BLU/GIA) have been supplemented with other good quality data from OCUO (76CHI/INA2, 76CHI/INA1, 74ATA/CHI) in the final correlation.

A large number of measurements (16 data sets) were performed in German laboratories (TUB, UMG, and UWG) before the World War II. The uncertainty of their data is 0.5 % or larger, especially for older measurements. These laboratories were particularly involved in investigations of deuterated compounds (38KRU/CLU, 47CLU/WOL), silane (33CLU), germane (42CLU/FAB), and hydrogen selenide (38KRU/CLU). The data for phosphine (36CLU/FRA1) have been supplemented by data from UCB (37STE/GIA). For a correlation of data for carbon monoxide, we have supplemented experimental data from the above German laboratories (16EUC, 29CLU1, 38KAI) with data from UCB (32CLA/GIA).

Very accurate and extensive measurements of four different fluorine compounds were carried out at WRUC (55PIE/PAC, 60BOC/PET, 62PAC/PET, 65PAC/TUR, 70PAC/JEP). Data for five chlorides were measured at ICG (86DEV/GUS, 87DEV/GUS, 87GIB/GUS, 87GUS/GIB, 87GUS/GUB); we have concluded that the real error in these data is about 0.5 %; this is an uncertainty about twice as large as that claimed by the authors.

The inorganic family includes several industrially important compounds. Heat capacity of carbon dioxide was measured up to the critical temperature at NBSB (86MAG/ELY); the reported uncertainty of the data is 0.5 % and seems to be realistic. The vapor pressure of carbon dioxide at the triple point temperature is about five times larger than the atmospheric pressure. Thus, all measurements in the liquid phase were carried out at an elevated pressure. Experimental data for nitrogen fluoride were also measured at NBSB (81WEB) as a function of temperature up to the vicinity of the critical temperature. The published data were the saturation heat capacities; as no *pVT* data were available for conversion to the isobaric heat capacity, all the presented recommended values relate to C_{sat}. These data have been supplemented for the correlation by the results from WRUC (55PIE/PAC); the average deviation between the two data sets is about 1 %.

For sulfur dioxide, we have jointly correlated data from two independent sources, UCB (38GIA/STE) and KITH (39RIE2), despite the fact that the heat capacity varied differently with temperature in these two sources. Due to the lack of information in the two original papers, it was impossible to decide which temperature dependence was closer to the reality. For that reason, we have assigned the level of uncertainty IV to the recommended data. For sulfur trioxide, we had only one primary set of calorimetric values in a very narrow temperature range (12 K) from The Kazan Institute of Chemical Technology (89KON/STR). We have opted, however, for secondary data on SO_3 published as parameters of a cubic equation in a review paper by (76MIL/SCH). As the primary data (obtained in US industrial laboratories) were unavailable to us, an exception has been made in the policy of not using secondary sources. The recommended data for sulfur trioxide have been assigned the level of uncertainty VI because information on the experimental procedure was not available.

Experimental data for carbon disulfide are very abundant. From 11 sets of data we have selected for the final correlation the data from UCB (37BRO/MAN), ICLO (55STA/TUP) and data generated from parameters of a quadratic equation published by Indian authors from IISB (70GOP/GAM).

Experimental data for hydrazine measured at BMB (49SCO/OLI) represent the only set of data from BMB for this family of compounds. We have supplemented these data by results from CITP (50HOU/MAS) for extending the BMB measurements towards higher temperatures, and with values reported by American Aviation, Inc., Canoga Park, California (68AHL/YOU).

Heat capacities of phosphoric acid have been calculated by us from heat capacity data on water solutions of phosphorus pentoxide, P_2O_5, published by Tennessee Valley Authority, Alabama (58EGA/LUF, 81LUF).

For the correlation of heat capacities of heavy water, the data from Queen Mary College, London (40COC/FER), UGG (51EUC/EIG) and the most extensive measurements published by U.S. Atomic Energy Commission (59BAK) have been selected from 9 available data sources.

The heat capacity of water was measured repeatedly (very often at the single temperature, 298.15 K) for verifying the reliability of a calorimeter. For this reason, we have not included all available sets in the table of experimental data. We have based our selection on two sets of data from NBSW (37OSB/STI, 39OSB/STI). The former set contains data measured up to the critical temperature with uncertainties between 1 to 1.5 %; the latter set contains highly accurate data (uncer-

tainty 0.1 %) from the melting temperature up to 368 K. Three data points in the proximity of the critical temperature were obviously subject to a large error and have been rejected from the final correlation. The above two sets from NBSW were supplemented with high precision data measured in the interval from 290 to 321 K at Queen Mary College, London (40COC/FER). For the conversion of C_{sat} to C_p, we have used the recent equation of state for water (84HAA/GAL).

Due to a frequent occurrence of a minimum on the $C_p=f(T)$ curve for many inorganic compounds, parameters of a quasi-polynomial equation either have not been calculated or were obtained for a limited temperature interval from the minimum on the curve to the upper temperature limit of the experimental data.

Name: Silver(1+) salt nitric acid
Formula: $AgNO_3$

CAS-RN: 7761-88-8
Group No.: 2-001
Molar Mass: 169.87

TABLE 2.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
07GUI2	N	502.1	1	nosp	not specified		C_{avg}	DSIO	07GUI2
09GOO/KAL	N	491.1–541.2	2	nosp	not specified		C_{avg}	DSIO	09GOO/KAL

07GUI2 average value in temperature range 481–523 K
09GOO/KAL constant value calculated from temperature dependence of enthalpy by the authors

TABLE 2.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
09GOO/KAL	491.1–541.2	2	3.00#	0.000	0.00	0.00	0.00	0
				Rejected data				
07GUI2	(6.84-1, 4.28, –6.84-1, –1)							

TABLE 2.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
491.1–541.2		1.66692+1					V

TABLE 2.1.4. Recommended values of heat capacities

Temp. (K)	500	540
c ($J K^{-1} g^{-1}$)	0.82	0.82
C ($J K^{-1} mol^{-1}$)	139	139

Name: Aluminium bromide
Formula: $AlBr_3$

CAS-RN: 7727-15-3
Group No.: 2-002
Molar Mass: 266.69

TABLE 2.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31FIS	N	370.6–407.1	2	nosp	not specified		C_p	DSTO	28FIS/BIL
69WEB/JUS	N	370.6–529.0	3	nosp	not specified		C_p	not specified	

31FIS constant value calculated from a graph (enthalpy versus temperature) by the compilers
69WEB/JUS data calculated by the authors from 31FIS

TABLE 2.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69WEB/JUS	370.6–529.0	3	3.00#	0.000	0.00	0.00	0.00	0
				Rejected data				
31FIS	(8.05–1, 5.08, 8.05–1, 2)							

TABLE 2.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	3	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
370.6–529.0		1.50311+1					VI

TABLE 2.2.4. Recommended values of heat capacities

Temp. (K)	370	450	530
c_p ($J K^{-1} g^{-1}$)	0.47	0.47	0.47
C_p ($J K^{-1} mol^{-1}$)	125	125	125

Name: Aluminium chloride
Formula: $AlCl_3$

CAS–RN: 7446–70–0
Group No.: 2–003
Molar Mass: 133.34

TABLE 2.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
31FIS	N	469.1–505.1	2	nosp	not specified	C_p	DSTO	28FIS/BIL

31FIS constant value calculated from a graph (enthalpy versus temperature) by the compilers

TABLE 2.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
469.1–505.1		1.74415+1					VI

TABLE 2.3.4. Recommended values of heat capacities

Temp. (K)	470	510
c_p ($J K^{-1} g^{-1}$)	1.09	1.09
C_p ($J K^{-1} mol^{-1}$)	145	145

Name: Aluminium iodide
Formula: AlI_3

CAS-RN: 7784-23-8
Group No.: 2-004
Molar Mass: 407.69

TABLE 2.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
31FIS N	464.1–480.1	2	nosp	not specified	C_p	DSTO	28FIS/BIL

31FIS constant value calculated from a graph (enthalpy versus temperature) by the compilers

TABLE 2.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
464.1–480.1	1.49908+1	V

TABLE 2.4.4. Recommended values of heat capacities

Temp. (K)	470	480
c_p ($J K^{-1} g^{-1}$)	0.31	0.31
C_p ($J K^{-1} mol^{-1}$)	125	125

Name: Arsenous trichloride
Formula: $AsCl_3$

CAS-RN: 7784-34-1
Group No.: 2-005
Molar Mass: 181.28

TABLE 2.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
87GIB/GUS	255.3–272.7	10	0.20	99.95 melpt	C_p	BSAO	86DEV/GUS

TABLE 2.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.213	6.97-3	0.04	5.34-6	1

Temp. range K	A_1	A_2	Level of uncertainty
255.3–272.7	1.67743+1	-1.55815-1	II

TABLE 2.5.4. Recommended values of heat capacities

Temp. (K)	260	270
c_p ($J K^{-1}g^{-1}$)	0.751	0.750
C_p ($J K^{-1}mol^{-1}$)	136.1	136.0

Name: Arsenous trifluoride
Formula: AsF_3

CAS–RN: 7784–35–2
Group No.: 2–006
Molar Mass: 131.92

TABLE 2.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41RUS/RUN	276.2–287.8	4	0.10	99.98	melpt	C_p	BSAO	41YOS/GAR

TABLE 2.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.733	1.11–2	0.07	7.63–6	0
Temp. range K		A_1	A_2				Level of uncertainty
276.2–287.8		1.37157+1	4.94961–1				II

TABLE 2.6.4. Recommended values of heat capacities

Temp. (K)	280	290
c_p ($J K^{-1}g^{-1}$)	0.952	0.955
C_p ($J K^{-1}mol^{-1}$)	125.6	126.0

Name: Arsine
Formula: AsH_3

CAS–RN: 7784–42–1
Group No.: 2–007
Molar Mass: 77.95

TABLE 2.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55SHE/GIA	160.9–207.6	8	nosp	99.96	melpt	C_p	BSIO	28GIA/WIE1

TABLE 2.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.262	5.72–3	0.08	5.25–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
160.9–207.6		8.58301	–1.47190	4.08470–1			II

TABLE 2.7.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210
c_p ($J K^{-1} g^{-1}$)	0.775	0.774	0.775	0.776	0.778
C_p ($J K^{-1} mol^{-1}$)	60.37	60.34	60.37	60.47	60.64

Name: Trifluoroborane
Formula: BF_3

CAS-RN: 7637-07-2
Group No.: 2-008
Molar Mass: 67.81

TABLE 2.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38EUC/SCH	145.0–173.0	5S	nosp	99.3	melpt	C_p	BSAO	38EUC/SCH

TABLE 2.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.032	2.83–3	0.02	7.63–7	0

Temp. range K	A_1	A_2	Level of uncertainty
145.0–173.0	1.08556+1	1.02776	IV

TABLE 2.8.4. Recommended values of heat capacities

Temp. (K)	150	160	170
c_p ($J K^{-1} g^{-1}$)	1.520	1.533	1.545
C_p ($J K^{-1} mol^{-1}$)	103.1	103.9	104.8

Name: Boron chloride (B_2Cl_4)
Formula: B_2Cl_4

CAS-RN: 13701-67-2
Group No.: 2-009
Molar Mass: 163.43

TABLE 2.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
58LIN/WAR	183.3–214.5	7	0.50	98.5	melpt	C_p	BSIO	36AST/MES

TABLE 2.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.440	3.65–2	0.22	1.14–4	–1

Temp. range K	A_1	A_2	Level of uncertainty
183.3–214.5	1.68135+1	–1.34233–1	IV

TABLE 2.9.4. Recommended values of heat capacities

Temp. (K)	190	200	210
c_p (J K^{-1}g^{-1})	0.842	0.842	0.841
C_p (J K^{-1}mol^{-1})	137.7	137.6	137.5

Name: Diborane (6)
Formula: B_2H_6

CAS–RN: 19287–45–7
Group No.: 2–010
Molar Mass: 27.67

TABLE 2.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53CLA/RIF	112.9–176.7	16	0.10	99.992	melpt	C_p	BSIO	50JOH/CLA
53RIF/KER	170.1–282.3	14	1.00	99.992	melpt	C_{sat}	BSIO	53RIF/KER

TABLE 2.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
53CLA/RIF	112.9–176.7	16	0.10	2.372	2.16–2	0.24	8.56–5	–2
53RIF/KER	170.–282.3	14	1.00	1.769	2.22–1	1.77	1.09–2	–2

TABLE 2.10.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	30	30	2.314	1.67–1	1.34	5.14–3	–4

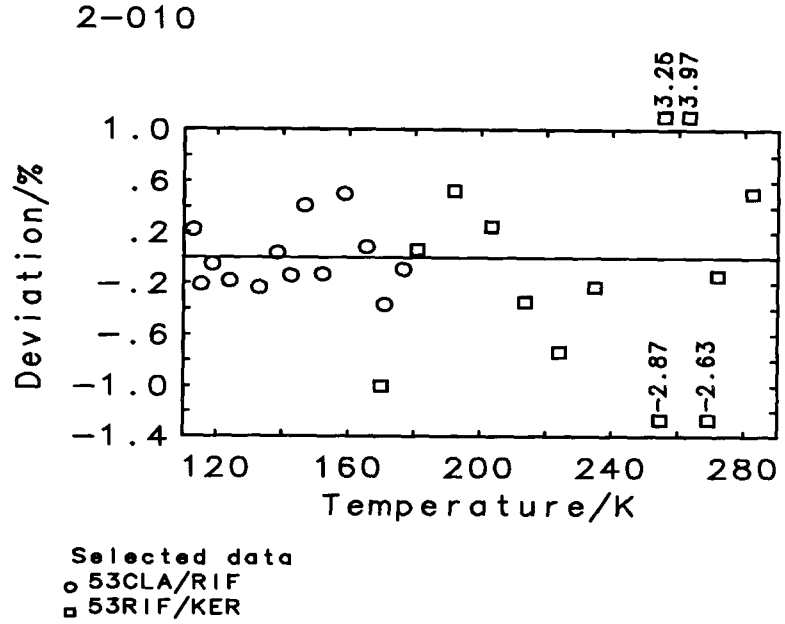
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
112.9–250.0	9.50739	6.57368–1	–1.63625	6.70162–1	IV
250.0–282.3	–3.26859+3	3.93437+3	–1.57512+3	2.10468+2	V

TABLE 2.10.4. Recommended values of heat capacities

Temp. (K)	110	120	130	140	150	160	170
c (J K^{-1}g^{-1})	2.747	2.734	2.725	2.722	2.727	2.739	2.761
C (J K^{-1}mol^{-1})	76.02	75.65	75.40	75.33	75.44	75.79	76.40
Temp. (K)	180	190	200	210	220	230	240
c (J K^{-1}g^{-1})	2.794	2.839	2.896	2.968	3.056	3.160	3.283
C (J K^{-1}mol^{-1})	77.30	78.54	80.14	82.13	84.56	87.45	90.83
Temp. (K)	250	260	270	273.15	280		
c (J K^{-1}g^{-1})	3.424	3.65	4.27	4.61	5.68		
C (J K^{-1}mol^{-1})	94.75	101	118	128	157		

TABLE 2.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	30	30	3.378	1.87-1	1.59	3.20-2	8
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
112.9–282.3	289.80	-2.22120	1.76504-1	7.70639	5.76824	-1.94083+1	1.16871+1	V



Name: Borazine
Formula: $B_3H_6N_3$

CAS-RN: 6569-51-3
Group No.: 2-011
Molar Mass: 80.50

TABLE 2.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91LEB/KUL	N	225.9–310.4	29	0.20	99.94	melpt	C_p	BSAO	76LEB/LIT

TABLE 2.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	29	29	1.092	7.31-2	0.44	5.76-4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
225.9–310.4		1.16116+1	1.32871-1	6.36502-1			III

TABLE 2.11.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.579	1.611	1.644	1.679	1.716	1.727	1.753
C_p ($J K^{-1}mol^{-1}$)	127.1	129.7	132.4	135.2	138.1	139.0	141.1
Temp. (K)	290	298.15	300	310			
c_p ($J K^{-1}g^{-1}$)	1.792	1.825	1.832	1.874			
C_p ($J K^{-1}mol^{-1}$)	144.3	146.9	147.5	150.8			

Name: Pentaborane(9)
Formula: B_5H_9

CAS-RN: 19624-22-7
Group No.: 2-012
Molar Mass: 63.13

TABLE 2.12.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
59WES2	N	298.15	2.373	nosp	not specified		C_p	not specified	

59WES2 unpublished data from Johnston H.L. et al.

Name: Decaborane (14)
Formula: $B_{10}H_{14}$

CAS-RN: 17702-41-9
Group No.: 2-013
Molar Mass: 122.22

TABLE 2.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
55FUR/PAR	373.0-380.0	6	0.30	99.984	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 2.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	6	6	1.272	1.44-1	0.38	1.81-4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
373.0-380.0		-5.97490+3	3.17983+3	-4.20378+2			III

TABLE 2.13.4. Recommended values of heat capacities

Temp. (K)	372	374	376	378	380
c_{sat} ($J K^{-1}g^{-1}$)	2.498	2.558	2.594	2.608	2.599
C_{sat} ($J K^{-1}mol^{-1}$)	305.3	312.6	317.1	318.8	317.7

Name: Hydrobromic acid–*d*
Formula: BrD

CAS–RN: 13536–59–9
Group No.: 2–014
Molar Mass: 81.92

TABLE 2.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47CLU/WOL	190.5–205.8	5	nosp	not specified		C_p	BSIO	36CLU/GOL
76CHI/INA2	187.6–188.2	2	0.20	99.927	melpt	C_p	BSAO	74ATA/CHI

TABLE 2.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CLU/WOL	190.5–205.8	5	0.50#	1.054	3.98–2	0.53	5.66–3	3
76CHI/INA2	187.6–188.2	2	0.20	1.942	2.91–2	0.39	–1.87–3	0

TABLE 2.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	1.809	4.90–2	0.65	3.51–3	3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
187.6–205.8	–2.10881	9.49143	–2.32871	IV

TABLE 2.14.4. Recommended values of heat capacities

Temp. (K)	190	200
c_p (J K^{-1}g^{-1})	0.763	0.767
C_p (J K^{-1}mol^{-1})	62.51	62.85

Name: Bromine fluoride (BrF_3)
Formula: BrF_3

CAS–RN: 7787–71–5
Group No.: 2–015
Molar Mass: 136.90

TABLE 2.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52OLI/GRI	285.5–308.1	8	0.20	99.91	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 2.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.525	1.57–2	0.10	2.50–5	0
Temp. range K		A_1	A_2				Level of uncertainty
285.5–308.1		1.30998+1	6.33129–1				II

TABLE 2.15.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	0.907	0.910	0.911	0.915
C_{sat} (J K^{-1}mol^{-1})	124.2	124.6	124.7	125.2

Name: Hydrobromic acid
Formula: BrH

CAS–RN: 10035–10–6
Group No.: 2–016
Molar Mass: 80.91

TABLE 2.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24EUC/KAR	190.7–198.3	4	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
28GIA/WIE2	189.9–205.1	6	0.30	not specified		C_{sat}	BSIO	28GIA/WIE1
76CHI/INA2	188.3–190.3	3	0.20	99.987	melpt	C_p	BSAO	74ATA/CHI

TABLE 2.16.2. Correlated heat capacities

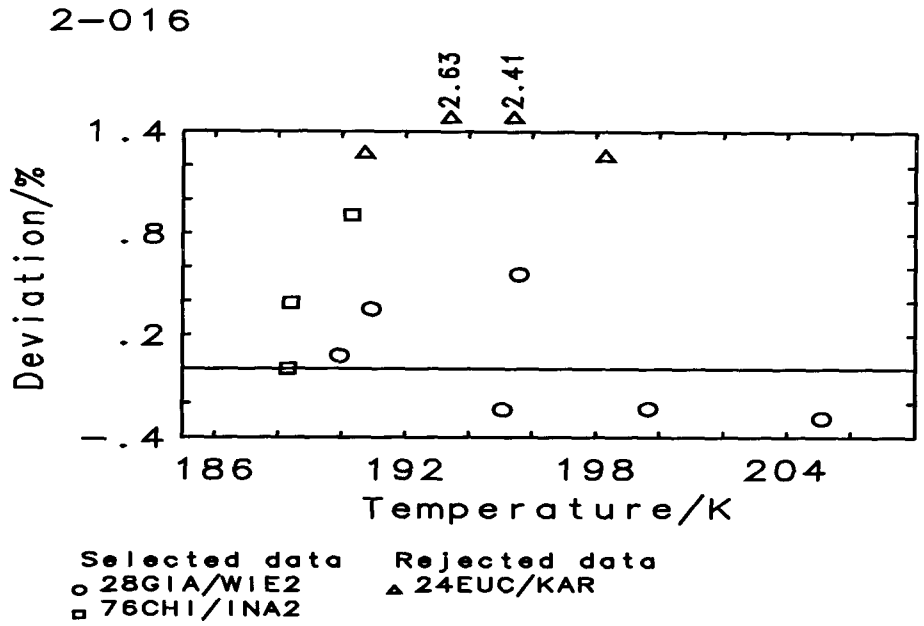
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
28GIA/WIE2	189.9–205.1	6	0.30	1.089	2.35–2	0.33	2.58–3	0
76CHI/INA2	188.3–190.3	3	0.20	4.853	6.89–2	0.97	–8.12–4	1
				Rejected data				
24EUC/KAR	(1.46–1, 1.99, 1.38–1, 4)							

TABLE 2.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	13	9	3.334	5.01–2	0.70	1.45–3	1
Temp. range K		A_1	A_2				Level of uncertainty
188.3–205.1		6.11645	5.39060–1				IV

TABLE 2.16.4. Recommended values of heat capacities

Temp. (K)	190	195	200	205
c ($J\,K^{-1}g^{-1}$)	0.734	0.737	0.739	0.742
C ($J\,K^{-1}mol^{-1}$)	59.37	59.60	59.82	60.04



Name: Indium bromide (InBr)
Formula: BrIn

CAS-RN: 14280-53-6
Group No.: 2-017
Molar Mass: 194.72

TABLE 2.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91GAR/PRE1	580.0–700.0	eqn	nosp	99.999	anal	C_p	BDHT	69PER/COM

TABLE 2.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	12	12	0.000	3.99-7	0.00	1.19-7	0
Temp. range K		A_1	A_2				Level of uncertainty
580.0–699.9		5.76462	2.36214-1				V

TABLE 2.17.4. Recommended values of heat capacities

Temp. (K)	580	600	620	640	660	680	700
c_p ($J K^{-1}g^{-1}$)	0.30	0.31	0.31	0.31	0.31	0.31	0.32
C_p ($J K^{-1}mol^{-1}$)	59.3	59.7	60.1	60.5	60.9	61.3	61.7

Name: Tin bromide ($SnBr_2$)
Formula: Br_2Sn

CAS–RN: 10031–24–0
Group No.: 2–018
Molar Mass: 278.52

TABLE 2.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91GAR/PRE2	520.0–800.0	eqn	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 2.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.000	6.48–7	0.00	–2.54–7	0

Temp. range K	A_1	A_2	Level of uncertainty
520.0–800.0	8.44067	6.01839–1	V

TABLE 2.18.4. Recommended values of heat capacities

Temp. (K)	520	540	560	580	600	620	640
c_p ($J K^{-1}g^{-1}$)	0.35	0.35	0.35	0.36	0.36	0.36	0.37
C_p ($J K^{-1}mol^{-1}$)	96.2	97.2	98.2	99.2	100	101	102
Temp. (K)	660	680	700	720	740	760	780
c_p ($J K^{-1}g^{-1}$)	0.37	0.37	0.38	0.38	0.38	0.39	0.39
C_p ($J K^{-1}mol^{-1}$)	103	104	105	106	107	108	109
Temp. (K)	800						
c_p ($J K^{-1}g^{-1}$)	0.40						
C_p ($J K^{-1}mol^{-1}$)	110						

Name: Tetrabromostannane
Formula: Br_4Sn

CAS–RN: 7789–67–5
Group No.: 2–019
Molar Mass: 438.33

TABLE 2.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
83BER/STE		306.9–336.2	8	nosp	99.98	melpt	C_p	BSAO	79AMI/LEB

36KUR/VOS average value in temperature range 290–333 K

TABLE 2.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83BER/STE	306.9–336.2	8	0.30#	0.142	8.35–3	0.04	7.15–6	–2
				Rejected data				
36KUR/VOS	(8.61, 30.50, 8.61, 1)							

TABLE 2.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	8	0.164	9.65–3	0.05	7.15–6	–2
Temp. range K		A_1	A_2				Level of uncertainty
306.9–336.2		2.17989+1	–6.98827–1				III

TABLE 2.19.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	0.372	0.371	0.370	0.368
C_p ($J K^{-1} mol^{-1}$)	163.2	162.7	162.1	161.5

Name: Carbonic dichloride
Formula: CCl_2O

CAS–RN: 75–44–5
Group No.: 2–020
Molar Mass: 98.92

TABLE 2.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48GIA/JON	148.4–279.4	24	nosp	99.993	melpt	C_p	BSIO	37GIA/EGA
60GIA/OTT	145.6–160.6	3	0.20	99.963	melpt	C_p	BSIO	37GIA/EGA

TABLE 2.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48GIA/JON	148.4–79.4	24	0.30#	0.525	1.90–2	0.16	–1.26–3	–4
60GIA/OTT	145.6–160.6	3	0.20	0.977	2.44–2	0.20	4.76–3	1

TABLE 2.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	27	0.642	2.13–2	0.18	–5.87–4	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
145.6–279.4		2.18191+1	–1.17651+1	4.58699	–5.79124–1		II

TABLE 2.20.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.054	1.039	1.028	1.019	1.013	1.009	1.007
C_p (J K^{-1}mol^{-1})	104.2	102.8	101.7	100.8	100.2	99.81	99.59
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.006	1.007	1.009	1.011	1.014	1.017	1.017
C_p (J K^{-1}mol^{-1})	99.53	99.59	99.76	99.99	100.3	100.6	100.6
Temp. (K)	280						
c_p (J K^{-1}g^{-1})	1.019						
C_p (J K^{-1}mol^{-1})	100.8						

Name: Carbonic difluoride
Formula: CF_2O

CAS–RN: 353–50–4
Group No.: 2–021
Molar Mass: 66.01

TABLE 2.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
68PAC/REN	165.9–187.9	10	0.10	99.85	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 2.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	1.815	2.41–2	0.18	5.96–5	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
165.9–187.9		–1.06008	1.81301+1	–5.64513			II

TABLE 2.21.4. Recommended values of heat capacities

Temp. (K)	170	180	190
c_{sat} (J K^{-1}g^{-1})	1.694	1.673	1.639
C_{sat} (J K^{-1}mol^{-1})	111.8	110.4	108.2

Name: Hydrocyanic acid
Formula: CHN

CAS-RN: 74-90-8
Group No.: 2-022
Molar Mass: 27.03

TABLE 2.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
39GIA/RUE	266.6–298.3	12	0.20	99.999	melpt	C_p	BSIO	37GIA/EGA

TABLE 2.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	12	12	1.528	2.60–2	0.31	1.32–4	2

Temp. range K	A_1	A_2	Level of uncertainty
266.6–298.3	8.12927	1.33473–1	III

TABLE 2.24.4. Recommended values of heat capacities

Temp. (K)	70	75	80	85
c_p ($J K^{-1}g^{-1}$)	2.138	2.152	2.167	2.182
C_p ($J K^{-1}mol^{-1}$)	59.87	60.28	60.70	61.11
c_{sat} ($J K^{-1}g^{-1}$)	2.138	2.149	2.161	2.172
C_{sat} ($J K^{-1}mol^{-1}$)	59.89	60.20	60.52	60.83

Name: Trithiocarbonic acid
Formula: CH_2S_3

CAS-RN: 594-08-1
Group No.: 2-023
Molar Mass: 110.22

TABLE 2.23.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity Method	Type capacity	Calorimeter Type	Calorimeter Reference
63GAT/KRE	N	272.15	1.347	nosp	not specified		C_{avg}	DSIO	63GAT/KRE

63GAT/KRE average value in temperature range 246–293 K

Name: Carbon monoxide
Formula: CO

CAS-RN: 630-08-0
Group No.: 2-024
Molar Mass: 28.01

TABLE 2.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
16EUC	69.3–77.9	4	nosp	not specified		C_{sat}	BSIO	16EUC
29CLU1	70.1–81.3	6	0.70	not specified		C_p	BSIO	29CLU1
32CLA/GIA	70.0–84.7	9	nosp	99.999	melpt	C_{sat}	BSIO	28GIA/WIE1
38KAI	70.9–75.8	10	0.40	not specified		C_p	BSIO	38KAI
66GIL/MOR	68.9–75.7	5	2.00	97.4	anal	C_p	BSAO	61FLU/LEA

TABLE 2.24.2. Correlated heat capacities

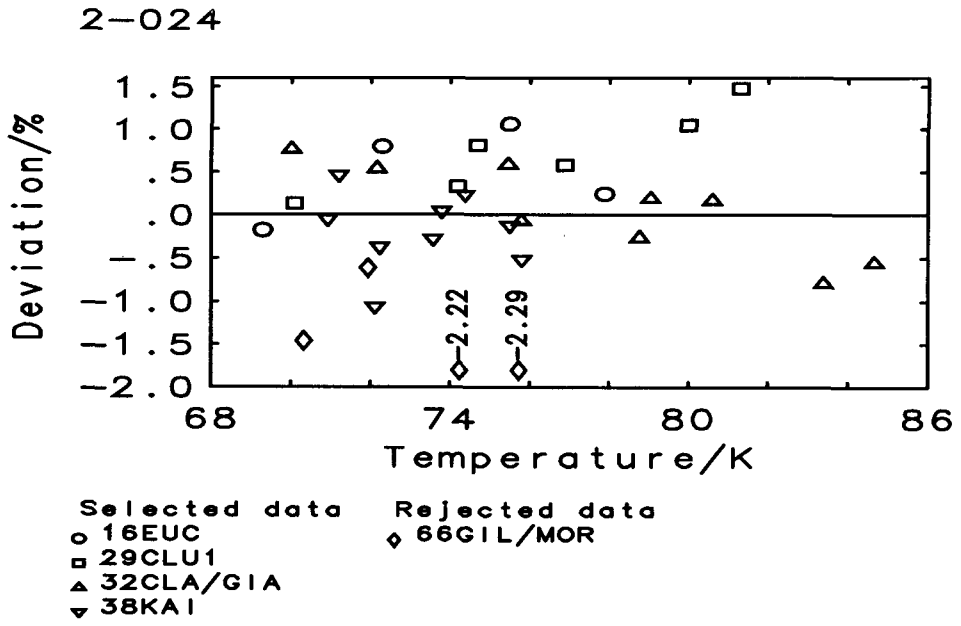
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
16EUC	69.3–77.9	4	1.00#	0.678	4.96–2	0.68	3.49–2	2
29CLU1	70.1–81.3	6	0.70	1.220	6.30–2	0.85	5.35–2	6
32CLA/GIA	70.0–84.7	9	0.60#	0.841	3.67–2	0.50	4.20–3	1
38KAI	70.9–75.8	10	0.40	1.108	3.18–2	0.44	–1.37–2	–4
				Rejected data				
66GIL/MOR	(1.27–1, 1.78, –1.17–1, –4)							

TABLE 2.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	29	1.044	4.55–2	0.62	1.25–2	5
C_{sat}	34	29	1.042	4.58–2	0.63	1.25–2	4
Temp. range K		A_1	A_2				Level of uncertainty
69.3–84.7		6.50679	9.91676–1				IV
69.3–84.7		6.67275	7.57508–1				IV

TABLE 2.24.4. Recommended values of heat capacities

Temp. (K)	70	75	80	85
c_p ($J K^{-1} g^{-1}$)	2.138	2.152	2.167	2.182
C_p ($J K^{-1} mol^{-1}$)	59.87	60.28	60.70	61.11
c_{sat} ($J K^{-1} g^{-1}$)	2.138	2.149	2.161	2.172
C_{sat} ($J K^{-1} mol^{-1}$)	59.89	60.20	60.52	60.83



Name: Carbon oxide sulfide
Formula: COS

CAS-RN: 463-58-1
Group No.: 2-025
Molar Mass: 60.08

TABLE 2.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37KEM/GIA	137.3–220.9	14	nosp	99.995	melpt	C_p	BSIO	28GIA/WIE1

TABLE 2.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.294	7.62–3	0.09	9.54–6	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
137.3–220.9	1.39741+1	–7.04145	2.89638	–3.68937–1	II

TABLE 2.25.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p ($J K^{-1} g^{-1}$)	1.215	1.202	1.192	1.185	1.181	1.179	1.180
C_p ($J K^{-1} mol^{-1}$)	73.01	72.20	71.60	71.19	70.94	70.85	70.88

Temp. (K)	210	220
c_p ($J K^{-1} g^{-1}$)	1.182	1.186
C_p ($J K^{-1} mol^{-1}$)	71.03	71.28

Name: Carbon dioxide
Formula: CO_2

CAS-RN: 124-38-9
Group No.: 2-026
Molar Mass: 44.01

TABLE 2.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26MAA/BAR	N	257.5	1	nosp	not specified		C_{avg}	DSIO	20MAA/HAT
28EUC/HAU		220.0–290.0	8S	nosp	not specified		C_{sat}	BSIO	28EUC/HAU
86MAG/ELY		220.4–303.0	77	0.50	99.9946	chrom	C_{sat}	BSAO	61GOO

26MAA/BAR average value in temperature range 217–298 K

TABLE 2.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86MAG/ELY	220.4–303.0	77	0.70#	0.883	1.70–1	0.62	2.25–3	–6
				Rejected data				
26MAA/BAR	(4.57–1, 4.05, –4.57–1, –1)			28EUC/HAU	(4.56–1, 4.18, –4.15–1, –7)			

TABLE 2.26.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	86	77	0.927	1.78–1	0.65	2.25–3	–6
C_{sat}	86	77	0.821	1.15–1	0.57	1.29–3	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
220.4–270.0	–1.78222+2	2.47707+2	–1.09285+2	1.62093+1	IV
270.0–290.0	–5.21131+3	5.84002+3	–2.18051+3	2.71916+2	IV
290.0–300.0	–2.20867+5	2.28932+5	–7.91088+4	9.11424+3	V
300.0–303.0	–2.68798+7	2.68879+7	–8.96543+6	9.96484+5	V
220.4–270.0	–1.03008+2	1.50085+2	–6.68718+1	1.00298+1	IV
270.0–290.0	–3.25145+3	3.64836+3	–1.36253+3	1.69987+2	IV
290.0–300.0	–1.21857+5	1.26343+5	–4.36711+4	5.03304+3	V
300.0–303.0	–1.40300+7	1.40345+7	–4.67972+6	5.20149+5	V

TABLE 2.26.4. Recommended values of heat capacities

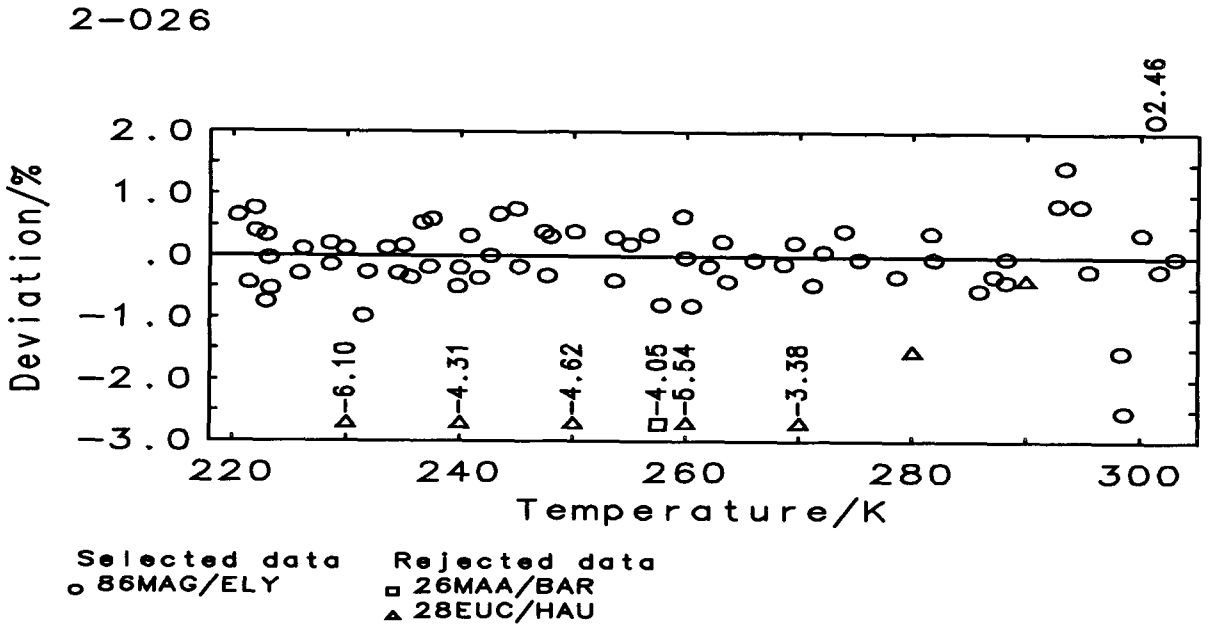
Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J\,K^{-1}g^{-1}$)	1.963	2.004	2.054	2.132	2.257	2.446	2.524
C_p ($J\,K^{-1}mol^{-1}$)	86.41	88.19	90.40	93.84	99.32	107.7	111.1
c_{sat} ($J\,K^{-1}g^{-1}$)	1.949	1.978	2.015	2.073	2.162	2.294	2.347
C_{sat} ($J\,K^{-1}mol^{-1}$)	85.78	87.04	88.69	91.22	95.15	101.0	103.3

Temp. (K)	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.767	3.480	5.47	6.56
C_p ($J\,K^{-1}mol^{-1}$)	121.8	153.1	241	289
c_{sat} ($J\,K^{-1}g^{-1}$)	2.511	2.974	4.17	4.80
C_{sat} ($J\,K^{-1}mol^{-1}$)	110.5	130.9	183	211

TABLE 2.26.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	86	77	1.384	3.99–1	0.97	–8.34–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
220.4–303.0	304.17	–3.85134	2.07142–1	–1.90613+1	1.25641+2	–1.90385+2	8.61326+1	V



Name: Carbon disulfide
Formula: CS_2

CAS-RN: 75-15-0
Group No.: 2-027
Molar Mass: 76.14

TABLE 2.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
07BAT	N	177.4–273.2	7	nosp	not specified	C_p	BSIO	07BAT
12SCH3		243.1–293.1	3	nosp	not specified	C_p	BSIO	12SCH1
25DRU/WEI		293.1	1	nosp	not specified	C_p	BSIO	25DRU/WEI
26SCH		288.1	1	nosp	not specified	C_p	not specified	
37BRO/MAN		163.9–297.4	18	nosp	99.999 melpt	C_p	BSIO	28LAT/GRE
39MAZ3	N	172.1–292.4	16	nosp	not specified	C_p	BSIO	39MAZ3
39PHI		301.1	1	nosp	not specified	C_p	BSIO	49WEI
45ZHD		280.4–304.3	3	nosp	not specified	C_p	BSIT	34KOL/UDO2
55STA/TUP		286.0–316.8	7	1.00	not specified	C_p	BSAO	55STA/TUP
71GAM/VIS	N	303.1–313.1	2	nosp	not specified	C_p	BSAO	71GOP/GAM
71GOP/GAM		303.0–320.0	eqn	1.00	not specified	C_p	BSAO	71GOP/GAM

07BAT same data in 08BAT
39MAZ3 data from a graph only
71GAM/VIS data from a graph only

TABLE 2.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37BRO/MAN	163.9–297.4	18	0.70#	1.009	6.44–2	0.71	–1.80–2	0
55STA/TUP	286.0–316.8	7	1.00	1.247	1.18–1	1.25	8.47–2	3
71GOP/GAM	303.0–320.2	5	1.00	0.670	6.41–2	0.67	2.52–2	1
				Rejected data				
07BAT	(1.22, 16.07, –1.10, –7)			12SCH3	(1.09–1, 1.21, –1.08–1, –3)			
25DRU/WEI	(4.48–2, 0.48, –4.48–2, –1)			26SCH	(5.89–1, 6.79, –5.89–1, –1)			
39MAZ3	(1.17, 15.51, –9.94–1, –14)			39PHI	(2.51–1, 2.74, –2.51–1, –1)			
45ZHD	(3.37–1, 3.76, –3.36–1, –3)			71GAM/VIS	(8.13–2, 0.85, 7.45–2, 2)			

TABLE 2.27.3. Parameters of regression polynomial

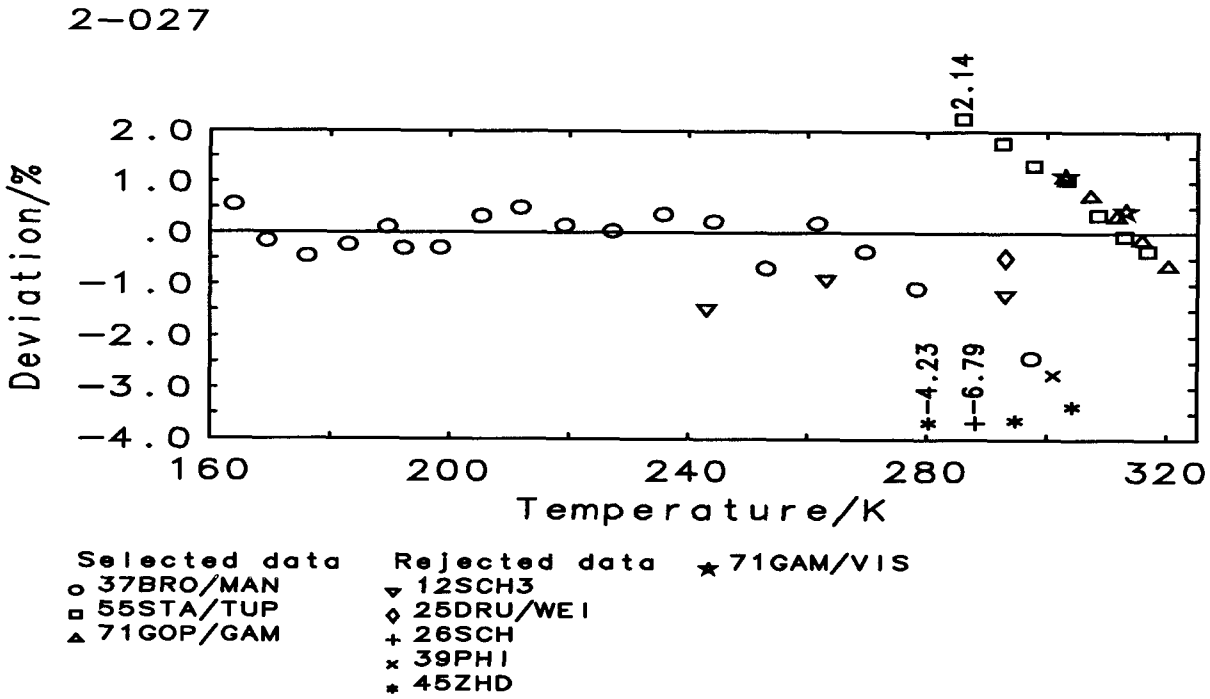
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	64	30	1.100	8.61–2	0.92	1.32–2	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
163.9–320.2		6.38046	4.30422	–2.26739	3.89181–1		IV

TABLE 2.27.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	0.989	0.988	0.987	0.986	0.985	0.985	0.985
C_p (J K^{-1}mol^{-1})	75.30	75.26	75.18	75.10	75.03	74.99	75.00
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	0.986	0.988	0.992	0.997	0.999	1.005	1.014
C_p (J K^{-1}mol^{-1})	75.08	75.25	75.53	75.93	76.09	76.49	77.21
Temp. (K)	298.15	300	310	320			
c_p (J K^{-1}g^{-1})	1.023	1.026	1.040	1.058			
C_p (J K^{-1}mol^{-1})	77.93	78.11	79.22	80.56			

TABLE 2.27.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	64	30	1.127	8.51–2	0.91	1.76–3	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
163.9–320.2	552.00	4.16496+1	1.38732+1	–5.31148	3.12597+1		V



Name: Carbon selenide (CSe_2)
Formula: CSe_2

CAS-RN: 506-80-9
Group No.: 2-028
Molar Mass: 169.93

TABLE 2.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
66GAT/DRA	233.1–323.1	10S	nosp	not specified		C_p	DSIO	63GAT/KRE

TABLE 2.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	1.108	9.37-2	0.89	1.35-3	0
Temp. range K		A_1	A_2				Level of uncertainty
233.1–323.1		7.82043	9.69064-1				IV

TABLE 2.28.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	0.492	0.496	0.501	0.506	0.511	0.512	0.515
C_p ($J K^{-1}mol^{-1}$)	83.55	84.36	85.17	85.97	86.78	87.03	87.58
Temp. (K)	290	298.15	300	310	320		
c_p ($J K^{-1}g^{-1}$)	0.520	0.524	0.525	0.530	0.534		
C_p ($J K^{-1}mol^{-1}$)	88.39	89.05	89.19	90.00	90.81		

Name: Nickel carbonyl
Formula: C_4NiO_4

CAS-RN: 13463-39-3
Group No.: 2-029
Molar Mass: 170.73

TABLE 2.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55SPI/STA	255.0–300.0	10S	0.50	99.99	melpt	C_p	BSAO	49STA/GUP

TABLE 2.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.020	2.42-3	0.01	1.14-6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
255.0–300.0		3.03711+1	-5.36978	1.15206			IV

TABLE 2.29.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.178	1.182	1.183	1.187	1.193	1.198	1.199
C_p ($J K^{-1}mol^{-1}$)	201.2	201.8	202.0	202.6	203.6	204.6	204.8

Name: Hydrochlorid acid-*d*
Formula: ClD

CAS-RN: 7698-05-7
Group No.: 2-030
Molar Mass: 37.47

TABLE 2.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47CLU/WOL	162.1–176.2	4	nosp	not specified		C_p	BSIO	36CLU/GOL
76CHI/INA1	160.7–162.9	2	0.20	99.976	melpt	C_p	BSAO	74ATA/CHI

TABLE 2.30.2. Correlated heat capacities

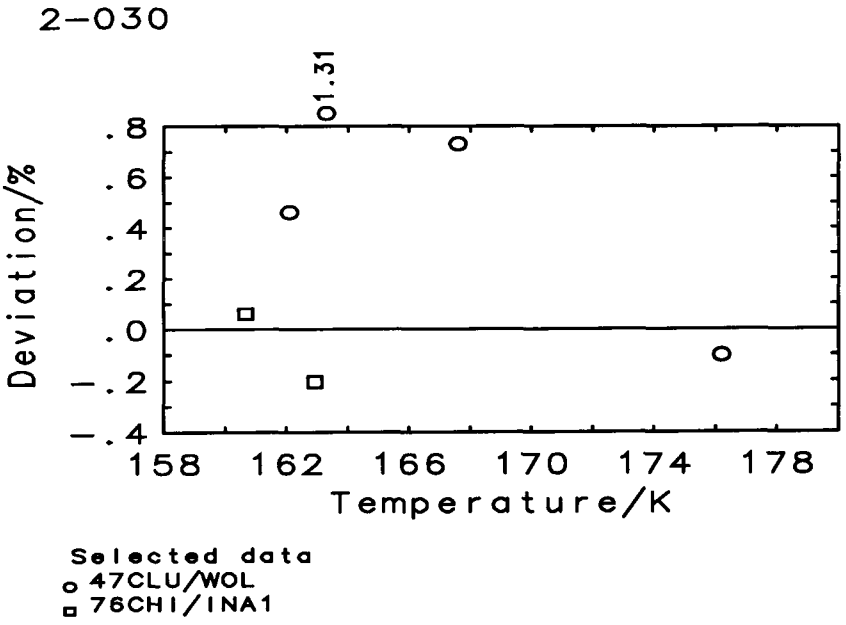
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CLU/WOL	162.1–176.2	4	0.80#	0.983	5.86–2	0.79	4.46–2	2
76CHI/INA1	160.7–162.9	2	0.20	0.759	1.11–2	0.15	–5.42–3	0

TABLE 2.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.120	5.91–2	0.79	2.79–2	2
Temp. range K		A_1	A_2				Level of uncertainty
160.7–176.2		6.46866	5.45731–1				IV

TABLE 2.30.4. Recommended values of heat capacities

Temp. (K)	160	170	180
c_p (J K^{-1}g^{-1})	1.629	1.641	1.653
C_p (J K^{-1}mol^{-1})	61.04	61.50	61.95



Name: Perchloryl fluoride ($(ClO_3)F$)
Formula: $ClFO_3$

CAS-RN: 7616-94-6
Group No.: 2-031
Molar Mass: 102.45

TABLE 2.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
58KOE/GIA	130.5–223.3	15	nosp	99.999	melpt	C_{sat}	BSIO	28GIA/WIE1

TABLE 2.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	15	15	0.426	9.21-3	0.09	1.14-5	-3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
130.5–223.3		1.15736+1	-1.83073	8.10623-1			II

TABLE 2.31.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J $K^{-1}g^{-1}$)	0.857	0.860	0.864	0.870	0.877	0.885	0.894
C_{sat} (J $K^{-1}mol^{-1}$)	87.83	88.13	88.56	89.13	89.83	90.67	91.64
Temp. (K)	200	210	220				
c_{sat} (J $K^{-1}g^{-1}$)	0.905	0.917	0.931				
C_{sat} (J $K^{-1}mol^{-1}$)	92.75	93.99	95.36				

TABLE 2.31.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	15	15	0.734	1.59-2	0.15	3.64-5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
130.5–223.3	368.00	2.29888	1.97504	8.25697	6.68955-1		II

Name: Chlorine fluoride (ClF_3)
Formula: ClF_3

CAS-RN: 7790-91-2
Group No.: 2-032
Molar Mass: 92.45

TABLE 2.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51GRI/BER	196.8–278.3	12	0.20	99.96	melpt	C_p	BSAO	43RUE/HUF

TABLE 2.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.268	7.30–3	0.05	5.80–6	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
196.8–278.3		1.41865+1	–1.22917	4.30487–1			II

TABLE 2.32.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.210	1.214	1.220	1.226	1.234	1.242	1.250
C_p (J K^{-1}mol^{-1})	111.8	112.3	112.8	113.4	114.0	114.8	115.6
Temp. (K)	270	273.15	280				
c_p (J K^{-1}g^{-1})	1.260	1.263	1.270				
C_p (J K^{-1}mol^{-1})	116.5	116.7	117.4				

Name: Hydrochlorid acid
Formula: ClH

CAS–RN: 7647–01–0
Group No.: 2–033
Molar Mass: 36.46

TABLE 2.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24EUC/KAR	164.3–188.2	9	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
28GIA/WIE1	163.7–185.2	5	nosp	not specified		C_p	BSIO	28GIA/WIE1
29CLU1	163.0–173.4	6	0.70	not specified		C_p	BSIO	29CLU1
76CHI/INA1	161.8–164.1	2	0.20	99.98	melpt	C_p	BSAO	74ATA/CHI

TABLE 2.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
28GIA/WIE1	163.7–185.2	5	0.50#	0.069	2.42–3	0.03	–1.17–3	–3
76CHI/INA1	161.8–164.1	2	0.20	0.065	9.13–4	0.01	4.71–4	1
				Rejected data				
24EUC/KAR	(5.27–1, 6.97, 5.25–1, 7)			29CLU1	(2.43–1, 3.35, 2.42–1, 6)			

TABLE 2.33.3. Parameters of regression polynomial

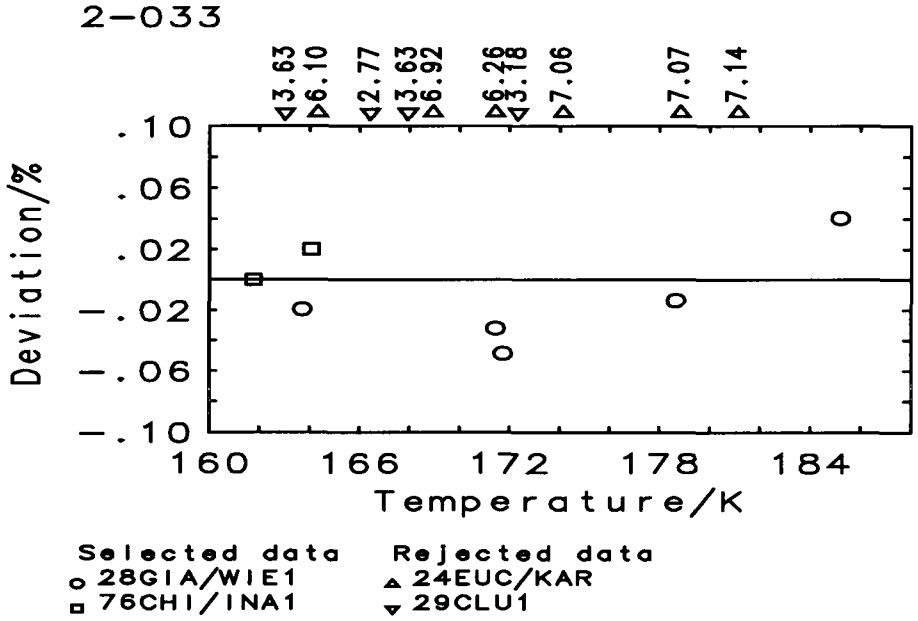
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	7	0.080	2.48–3	0.04	–7.04–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
161.8–185.2		6.33282	4.02127–1				III

TABLE 2.33.4. Recommended values of heat capacities

Temp. (K)	160	165	170	175	180	185
c_p ($J K^{-1}g^{-1}$)	1.591	1.595	1.600	1.605	1.609	1.614
C_p ($J K^{-1}mol^{-1}$)	58.00	58.17	58.34	58.51	58.67	58.84

TABLE 2.33.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	22	7	0.078	1.27–3	0.02	–6.34–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
161.8–185.2	324.70	5.96279–2	3.15811–1	6.39398	2.81457–3		III



Name: Perchloric acid
Formula: $ClHO_4$

CAS-RN: 7601–90–3
Group No.: 2–034
Molar Mass: 100.46

TABLE 2.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
64TRO/WES1	173.3–295.1	20	0.10	97.5	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 2.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	20	20	1.544	2.10–2	0.15	5.58–5	–4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
173.3–295.1		1.31461+1	–7.18856–1	3.97487–1			II

TABLE 2.34.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.088	1.094	1.101	1.108	1.116	1.125	1.135
C_{sat} (J K^{-1}mol^{-1})	109.3	109.9	110.6	111.3	112.1	113.0	114.0
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.145	1.156	1.167	1.171	1.179	1.192	1.203
C_{sat} (J K^{-1}mol^{-1})	115.0	116.1	117.3	117.6	118.5	119.8	120.9
Temp. (K)	300						
c_{sat} (J K^{-1}g^{-1})	1.206						
C_{sat} (J K^{-1}mol^{-1})	121.1						

Name: Iodine chloride
Formula: ClI

CAS-RN: 7790-99-0
Group No.: 2-035
Molar Mass: 162.36

TABLE 2.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*92STO	N	318.8	1	nosp	not specified		C_{avg}	DSIO	*92STO
65CAL/GIA		303.7–317.8	3	nosp	99.99	melpt	C_p	BSIO	37GIA/EGA

*92STO average value in temperature range 288–350 K

TABLE 2.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_T C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
65CAL/GIA	303.7–317.8	3	0.30#	0.443	1.65–2	0.13	4.42–5	–1

TABLE 2.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	3	0.768	2.86–2	0.23	4.42–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
303.7–317.8		1.26430+1	–7.79397–2				III

TABLE 2.35.4. Recommended values of heat capacities

Temp. (K)	305	310	315
c_p ($J K^{-1} g^{-1}$)	0.635	0.635	0.635
C_p ($J K^{-1} mol^{-1}$)	103.1	103.1	103.1

Name: Sodium salt chloric acid
Formula: $ClNaO_3$

CAS–RN: 7775–09–9
Group No.: 2–036
Molar Mass: 106.44

TABLE 2.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
09GOO/KAL	N	528.2–572.2	2	nosp	not specified		C_{avg}	DSIO	09GOO/KAL

09GOO/KAL constant value calculated from temperature dependence of enthalpy by the authors

TABLE 2.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
528.2–572.2	1.74079+1	V

TABLE 2.36.4. Recommended values of heat capacities

Temp. (K)	530	570
c ($J K^{-1} g^{-1}$)	1.36	1.36
C ($J K^{-1} mol^{-1}$)	145	145

Name: Thionyl chloride
Formula: Cl_2OS

CAS–RN: 7719–09–7
Group No.: 2–037
Molar Mass: 118.97

TABLE 2.37.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity Method	Type capacity	Calorimeter Type	Calorimeter Reference
*82OGI	N	311.65	1.015	nosp	not specified		C_{avg}	DSIO	*79BER

*82OGI average value in temperature range 290–333 K

Name: Sulfuryl chloride
Formula: Cl_2O_2S

CAS-RN: 7791-25-5
Group No.: 2-038
Molar Mass: 134.97

TABLE 2.38.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
*82OGI	N	312.15	0.9749	nosp	not specified		C_{avg}	DSIO	*79BER

*82OGI average value in temperature range 288–336 K

Name: Disulfuryl chloride
Formula: $Cl_2O_5S_2$

CAS-RN: 7791-27-7
Group No.: 2-039
Molar Mass: 215.03

TABLE 2.39.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
*82OGI	N	345.65	1.079	nosp	not specified		C_{avg}	DSIO	*79BER

*82OGI average value in temperature range 288–403 K

Name: Sulfur chloride (S_2Cl_2)
Formula: Cl_2S_2

CAS-RN: 10025-67-9
Group No.: 2-040
Molar Mass: 135.04

TABLE 2.40.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
*81OGI	N	314.15	0.9205	nosp	not specified		C_{avg}	DSIO	*79BER

*81OGI average value in temperature range 285–343 K

Name: Tin chloride ($SnCl_2$)
Formula: Cl_2Sn

CAS-RN: 7772-99-8
Group No.: 2-041
Molar Mass: 189.62

TABLE 2.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91GAR/PRE2	520.0–800.0	eqn	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 2.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.000	5.29–7	0.00	2.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
520.0–800.0		8.86042	4.87220–1				V

TABLE 2.41.4. Recommended values of heat capacities

Temp. (K)	520	560	600	640	680	720	760
c_p (J K^{-1}g^{-1})	0.50	0.51	0.52	0.53	0.53	0.54	0.55
C_p (J K^{-1}mol^{-1})	94.7	96.4	98.0	99.6	101	103	104
Temp. (K)	800						
c_p (J K^{-1}g^{-1})	0.56						
C_p (J K^{-1}mol^{-1})	106						

Name: Trichlorosilane
Formula: Cl_3HSi

CAS–RN: 10025–78–2
Group No.: 2–042
Molar Mass: 135.45

TABLE 2.42.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
66TEC	N	315.65	0.9623	nosp	not specified		C_{avg}	not specified	

66TEC average value in temperature range 298–333K

Name: Phosphoryl chloride
Formula: Cl_3OP

CAS–RN: 10025–87–3
Group No.: 2–043
Molar Mass: 153.33

TABLE 2.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
60OTT/GIA	280.9–300.2	6	nosp	99.98	melpt	C_p	BSIO	28GIA/WIE1

TABLE 2.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.484	1.61–2	0.10	2.07–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
280.9–300.2		1.51391+1	5.18557–1				II

TABLE 2.43.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	0.900	0.902	0.905	0.905
C_p ($J\,K^{-1}mol^{-1}$)	137.9	138.4	138.7	138.8

Name: Phosphorous trichloride
Formula: Cl_3P

CAS-RN: 7719-12-2
Group No.: 2-044
Molar Mass: 137.33

TABLE 2.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87DEV/GUS	186.2–272.5	25	0.20	99.999	chrom	C_p	BSAO	86DEV/GUS

TABLE 2.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	0.386	1.14–2	0.08	1.64–5	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
186.2–272.5		2.22974+1	–1.00511+1	4.27091	–5.81474–1		II

TABLE 2.44.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J\,K^{-1}g^{-1}$)	0.890	0.887	0.886	0.886	0.886	0.888	0.890
C_p ($J\,K^{-1}mol^{-1}$)	122.2	121.8	121.6	121.6	121.7	121.9	122.2
Temp. (K)	240	250	260	270			
c_p ($J\,K^{-1}g^{-1}$)	0.892	0.895	0.897	0.899			
C_p ($J\,K^{-1}mol^{-1}$)	122.5	122.9	123.2	123.5			

TABLE 2.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	0.517	1.53–2	0.10	2.84–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
186.2–272.5	563.00	1.04426+1	4.68709	9.88347	5.81639		II

Name: Tetrachlorogermane
Formula: Cl_4Ge

CAS–RN: 10038–98–9
Group No.: 2–045
Molar Mass: 214.42

TABLE 2.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86DEV/GUS	221.7–273.1	7S	0.20	99.991	melpt	C_{sat}	BSAO	86DEV/GUS

TABLE 2.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.082	2.83–3	0.02	2.72–7	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
221.7–273.1	1.46572+1	1.95136	–3.52805–1	II

TABLE 2.45.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270
c_{sat} (J $K^{-1}g^{-1}$)	0.670	0.671	0.672	0.673	0.673
C_{sat} (J $K^{-1}mol^{-1}$)	143.7	143.9	144.1	144.2	144.3

Name: Tetrachlorosilane
Formula: Cl_4Si

CAS–RN: 10026–04–7
Group No.: 2–046
Molar Mass: 169.90

TABLE 2.46.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
08KAH/KOE	N	303.1	1	nosp	not specified		C_{avg}	DSIO	01KAH
22LAT		208.8–294.3	2	2.00	not specified		C_p	BSIO	20GIB/LAT
37VOL		298.1	1	nosp	not specified		C_p	BSIO	37VOL
66SAV		293.0–323.0	eqn	1.20	not specified		C_p	BSIO	66SAV
74WIL/ZET		273.1–323.1	6S	nosp	not specified		C_p	BSAO	64ARN1
87GUS/GIB		205.4–272.1	16	0.20	99.995	chrom	C_p	BSAO	86DEV/GUS

08KAH/KOE average value in temperature range 293–313 K

TABLE 2.46.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74WIL/ZET	273.1–323.1	6	0.80#	2.699	3.61–1	2.16	2.46–1	4
87GUS/GIB	205.4–272.1	16	0.40#	1.306	8.27–2	0.52	–2.07–2	0
				Rejected data				
08KAH/KOE	(3.45–1, 2.12, –3.45–1, –1)			22LAT	(1.07, 6.19, 1.06, 2)			
37VOL	(6.59–1, 3.84, 6.59–1, 1)			66SAV	(1.60, 8.48, 1.46, 6)			

TABLE 2.46.3. Parameters of regression polynomial

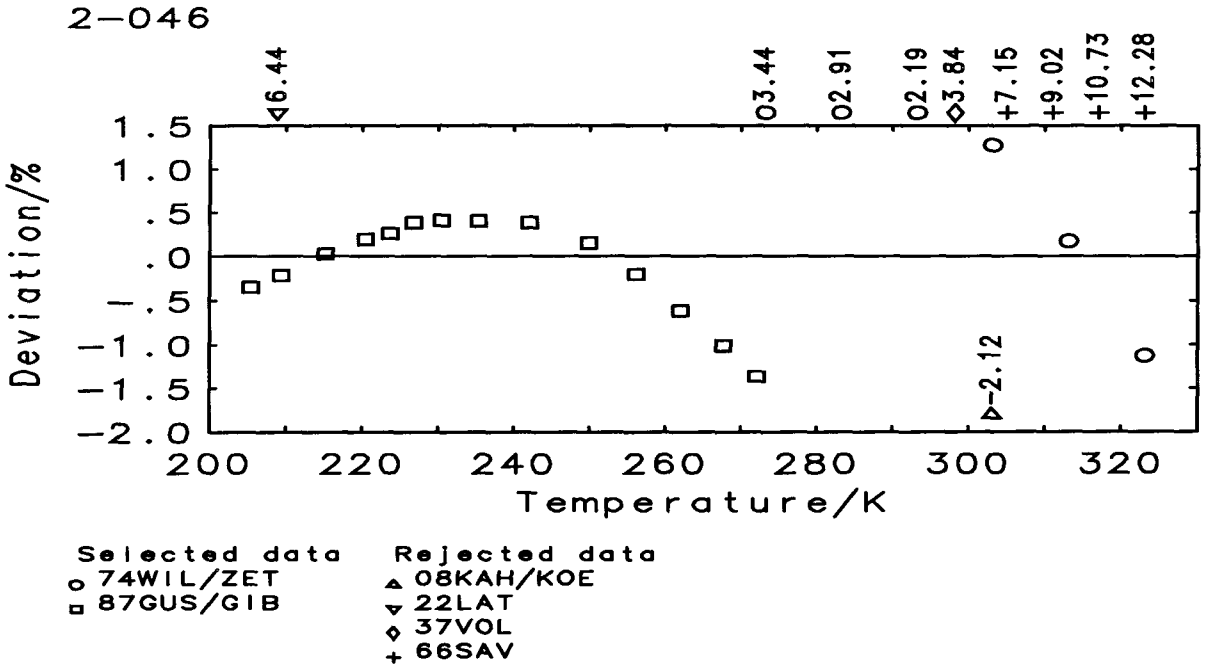
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	22	1.933	2.16–1	1.30	5.20–2	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
205.4–323.1		2.48455+1	–7.81485	1.68321			V

TABLE 2.46.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1} g^{-1}$)	0.78	0.77	0.77	0.77	0.77	0.78	0.78
C_p ($J K^{-1} mol^{-1}$)	132	131	131	131	132	132	133
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p ($J K^{-1} g^{-1}$)	0.79	0.79	0.80	0.81	0.81	0.82	0.84
C_p ($J K^{-1} mol^{-1}$)	134	134	136	137	138	140	142

TABLE 2.46.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R		s_r %	s_b/R	+/–
C_p	32	22	2.729	2.21–1		1.36	2.91–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4			Level of uncertainty
205.4–323.1	506.70	9.16339	4.65359	1.07622+1	4.51090			V



Name: Tetrachlorostannane
Formula: Cl_4Sn

CAS–RN: 7646–78–8
Group No.: 2–047
Molar Mass: 260.52

TABLE 2.47.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
22LAT		266.1–294.0	2	2.00	not specified		C_p	BSIO	20GIB/LAT
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
37VOL		298.1	1	nosp	not specified		C_p	BSIO	37VOL
74WIL/ZET		273.1–323.1	6	nosp	not specified		C_p	BSAO	64ARN1
84BER/STE		243.3–327.3	18	nosp	99.95	melpt	C_p	BSAO	79AMI/LEB
87GUS/GIB		242.4–272.1	13	0.20	99.995	chrom	C_p	BSAO	86DEV/GUS

36KUR/VOS average value in temperature range 290–333 K

TABLE 2.47.2. Correlated heat capacities

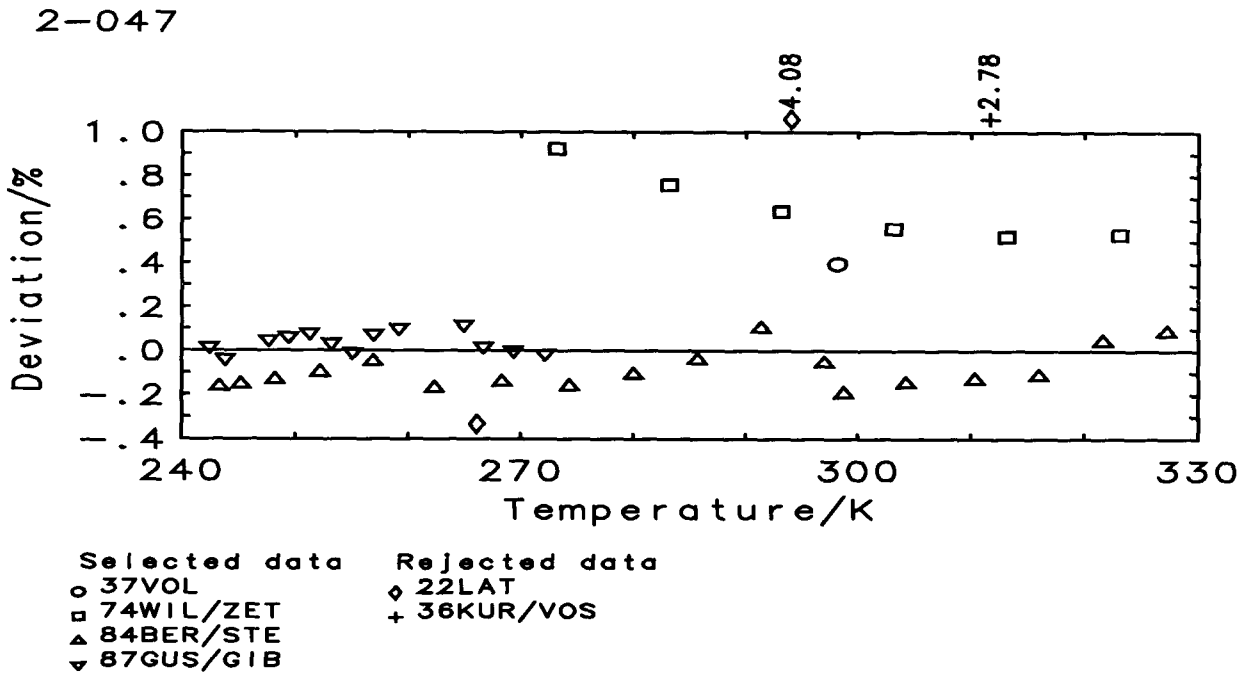
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37VOL	298.1	1	0.80#	0.495	7.54–2	0.40	7.54–2	1
74WIL/ZET	273.1–323.1	6	0.80#	0.837	1.28–1	0.67	1.25–1	6
84BER/STE	243.3–327.3	18	0.30#	0.425	2.42–2	0.13	–1.77–2	–12
87GUS/GIB	242.4–272.1	13	0.20	0.294	1.13–2	0.06	7.05–3	6
				Rejected data				
22LAT	(5.72–1, 2.89, 3.71–1, 0)			36KUR/VOS	(5.40–1, 2.78, 5.40–1, 1)			

TABLE 2.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	38	0.502	5.76–2	0.30	1.57–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
242.4–327.3		1.68997+1	1.94005	–4.20380–1			III

TABLE 2.47.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J\,K^{-1}g^{-1}$)	0.611	0.610	0.610	0.609	0.608	0.608	0.606
C_p ($J\,K^{-1}mol^{-1}$)	159.1	159.0	158.8	158.6	158.5	158.3	157.9
Temp. (K)	298.15	300	310	320	330		
c_p ($J\,K^{-1}g^{-1}$)	0.605	0.604	0.602	0.600	0.598		
C_p ($J\,K^{-1}mol^{-1}$)	157.5	157.4	156.9	156.3	155.7		



Name: Tellurium chloride ($TeCl_4$)
Formula: Cl_4Te

CAS–RN: 10026–07–0
Group No.: 2–048
Molar Mass: 269.41

TABLE 2.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
38FRE/HIL2	N	497.3–538.2	2	1.00	not specified	C_{avg}	DSIO	38FRE/HIL1

38FRE/HIL2 constant value calculated from temperature dependence of enthalpy by the authors

TABLE 2.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
497.3–538.2		2.76769+1					V

TABLE 2.48.4. Recommended values of heat capacities

Temp. (K)	500	540
c ($J K^{-1} g^{-1}$)	0.85	0.85
C ($J K^{-1} mol^{-1}$)	230	230

Name: Titanium chloride ($TiCl_4$)
Formula: Cl_4Ti

CAS–RN: 7550–45–0
Group No.: 2–049
Molar Mass: 189.69

TABLE 2.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
22LAT	251.6–294.3	2	2.00	not specified		C_p	BSIO	20GIB/LAT
66SAV	293.5–331.4	7	1.20	not specified		C_p	BSIO	66SAV

TABLE 2.49.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
66SAV	293.5–331.4	7	1.20	0.195	4.49–2	0.23	2.65–4	1
				Rejected data				
22LAT	(4.31–1, 2.34, 4.31–1, 1)							

TABLE 2.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	7	0.230	5.31–2	0.28	2.65–4	1
Temp. range K		A_1	A_2				Level of uncertainty
293.5–331.4		–4.63803	7.68756				V

TABLE 2.49.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	0.77	0.80	0.81	0.84	0.87	0.91
C_p ($J\,K^{-1}mol^{-1}$)	147	152	153	160	166	172

Name: Cesium fluoride ($Cs(HF_2)$)
Formula: CsF_2H

CAS–RN: 12280–52–3
Group No.: 2–050
Molar Mass: 171.91

TABLE 2.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78WES/LAN	460.9–528.4	10	nosp	99.92	melpt	C_p	BSAO	68WES/WES

TABLE 2.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.427	2.40–2	0.17	6.54–5	0
Temp. range K		A_1	A_2				Level of uncertainty
460.9–528.4		1.16474+1	5.03795–1				III

TABLE 2.50.4. Recommended values of heat capacities

Temp. (K)	460	470	480	490	500	510	520
c_p ($J K^{-1}g^{-1}$)	0.675	0.678	0.680	0.683	0.685	0.688	0.690
C_p ($J K^{-1}mol^{-1}$)	116.1	116.5	116.9	117.4	117.8	118.2	118.6
Temp. (K)	530						
c_p ($J K^{-1}g^{-1}$)	0.692						
C_p ($J K^{-1}mol^{-1}$)	119.0						

Name: Deuterium molecule with hydrogen
Formula: DH

CAS–RN: 13983–20–5
Group No.: 2–051
Molar Mass: 3.02

TABLE 2.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48WOO/SCO	N	16.6–22.0	7S	nosp	not specified		C_{sat}	not specified	

48WOO/SCO unpublished data measured by F.G. Brickwedde and R.B. Scott

TABLE 2.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	7	7	0.398	5.32–3	0.20	1.03–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
16.6–22.0		–1.54338	2.78828+1	–3.16203+1			IV

TABLE 2.51.4. Recommended values of heat capacities

Temp. (K)	17	18	19	20	21	22
c_{sat} ($J K^{-1}g^{-1}$)	6.281	6.744	7.189	7.617	8.027	8.420
C_{sat} ($J K^{-1}mol^{-1}$)	18.98	20.38	21.72	23.02	24.26	25.45

Name: Hydroiodic acid–*d*
Formula: DI

CAS–RN: 14104–45–1
Group No.: 2–052
Molar Mass: 128.92

TABLE 2.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
47CLU/WOL	224.8–227.7	3	nosp	not specified	C_p	BSIO	36CLU/GOL
78INA/CHI	223.3	1	0.20	99.994 melpt	C_p	BSAO	74ATA/CHI

TABLE 2.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CLU/WOL	224.8–227.7	3	0.50#	2.331	9.09–2	1.16	3.54–2	1
78INA/CHI	223.3	1	0.40#	2.071	6.30–2	0.83	–6.30–2	–1

TABLE 2.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	3.208	1.20–1	1.54	1.08–2	0
Temp. range K		A_1	A_2				Level of uncertainty
223.3–227.7		3.59995–1	3.26943				V

TABLE 2.52.4. Recommended values of heat capacities

Temp. (K)	223	225	227
c_p ($J\,K^{-1}g^{-1}$)	0.49	0.50	0.50
C_p ($J\,K^{-1}mol^{-1}$)	63.6	64.2	64.7

Name: Water-d_2
Formula: D_2O

CAS-RN: 7789-20-0
Group No.: 2-053
Molar Mass: 20.03

TABLE 2.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
35BAR/CLU	N	284.1	1	1.00	99.7	anal	C_{avg}	DSTO	35BAR/CLU
35BRO/BAR1	N	287.6	1	1.00	98.	anal	C_{avg}	DSAO	30BAR/MAA
35BRO/BAR2	N	288.1-318.6	3	1.00	98.	anal	C_{avg}	DSAO	30BAR/MAA
35JAC	N	276.9	1	nosp	97.7	anal	C_{sat}	BSIO	35JAC
36LON/KEM		279.4-295.2	4	0.20	99.997	melpt	C_p	BSIO	36GIA/STO
40COC/FER	N	285.1-325.8	31	nosp	99.2	anal	C_{sat}	BDHO	40COC/FER
51EUC/EIG	N	293.0-398.0	12S	nosp	96.	estim	C_{sat}	BSAO	51EUC/EIG
59BAK	N	304.0-473.1	37	nosp	99.77	anal	C_{sat}	BSIO	59BAK
70KRE		298.1	1	nosp	99.7	anal	C_p	BSAO	63BEN

35BAR/CLU average value in temperature range 277-291 K
35BRO/BAR1 average value in temperature range 277-298 K
35BRO/BAR2 average values in temperature ranges 277-299 K, 299-318 K and 299-338 K
35JAC value extrapolated to 100 % D2O
40COC/FER preliminary data published in 36FER/COC
51EUC/EIG purity was estimated from density by the authors
59BAK data in temperature range 373-473 K measured in an isoperibol calorimeter (but not described)

TABLE 2.53.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
40COC/FER	285.1-325.8	31	0.50#	0.276	1.40-2	0.14	1.99-3	-3
51EUC/EIG	293.0-398.0	11	0.30#	0.490	1.48-2	0.15	-9.00-3	-7
59BAK	304.0-473.1	37	0.70#	1.068	7.55-2	0.75	1.28-2	2
70KRE	298.1	1	0.30#	0.050	1.51-3	0.01	-1.51-3	-1
				Rejected data				
35BRO/BAR1	(2.03-1, 1.96, 2.03-1, 1)			35BRO/BAR2	(7.08-2, 0.69, 5.34-2, 1)			
36LON/KEM	(1.53-1, 1.54, -1.47-1, -2)							

TABLE 2.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	91	80	0.788	5.37-2	0.53	5.42-3	-9
C_{sat}	91	80	0.788	5.37-2	0.53	5.48-3	-11

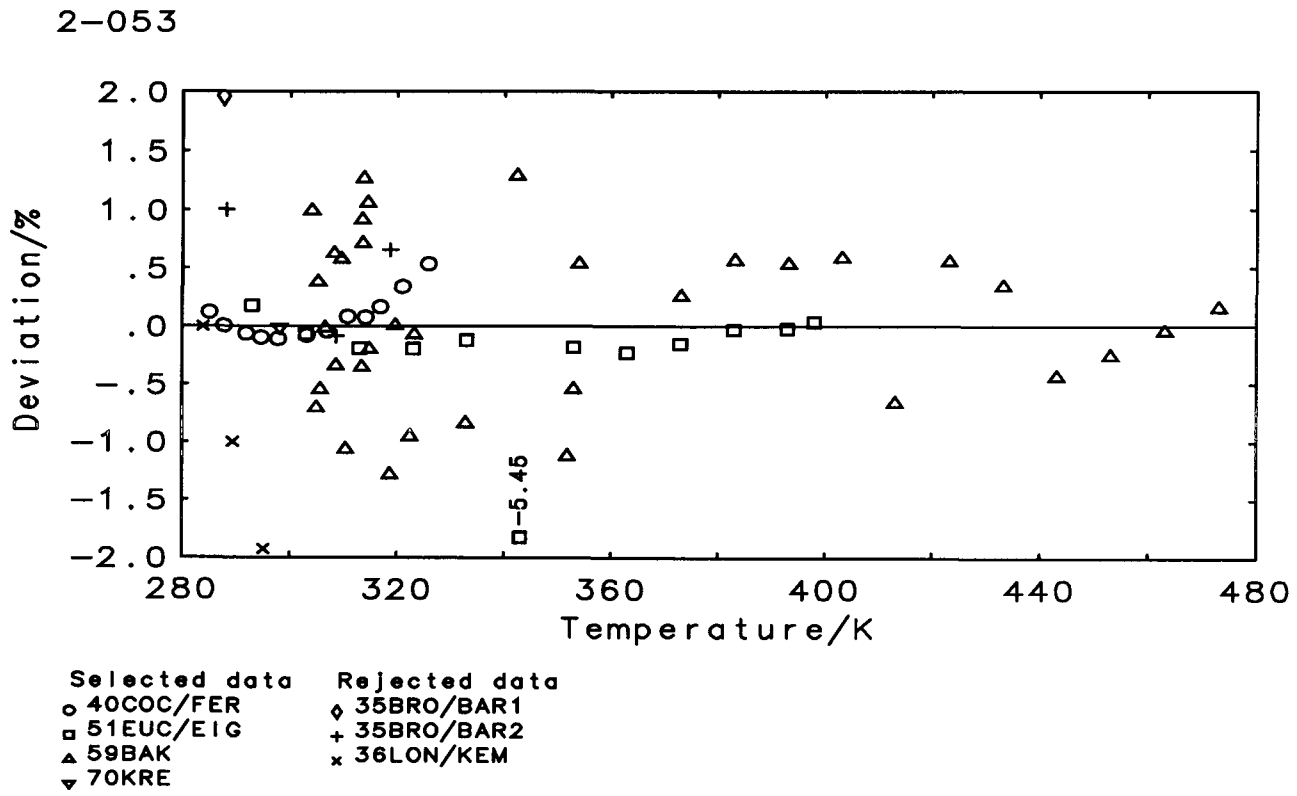
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
285.1-473.1	1.15134	8.71318	-2.74578	2.79911-1	IV
285.1-473.1	1.69083	8.21175	-2.59048	2.63876-1	IV

TABLE 2.53.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	4.220	4.216	4.210	4.208	4.199	4.188	4.177
C_p ($J\,K^{-1}mol^{-1}$)	84.52	84.43	84.31	84.28	84.09	83.88	83.66
c_{sat} ($J\,K^{-1}g^{-1}$)	4.221	4.216	4.210	4.208	4.199	4.188	4.177
C_{sat} ($J\,K^{-1}mol^{-1}$)	84.53	84.43	84.31	84.28	84.09	83.88	83.66
Temp. (K)	**340**	**350**	**360**	**370**	**380**	**390**	**400**
c_p ($J\,K^{-1}g^{-1}$)	4.167	4.157	4.149	4.143	4.140	4.141	4.146
C_p ($J\,K^{-1}mol^{-1}$)	83.45	83.25	83.09	82.97	82.91	82.92	83.03
c_{sat} ($J\,K^{-1}g^{-1}$)	4.167	4.157	4.148	4.142	4.138	4.138	4.142
C_{sat} ($J\,K^{-1}mol^{-1}$)	83.45	83.25	83.08	82.95	82.88	82.88	82.96
Temp. (K)	**410**	**420**	**430**	**440**	**450**	**460**	**470**
c_p ($J\,K^{-1}g^{-1}$)	4.156	4.172	4.194	4.224	4.262	4.308	4.363
C_p ($J\,K^{-1}mol^{-1}$)	83.23	83.55	84.00	84.60	85.35	86.28	87.39
c_{sat} ($J\,K^{-1}g^{-1}$)	4.151	4.166	4.186	4.213	4.248	4.291	4.342
C_{sat} ($J\,K^{-1}mol^{-1}$)	83.14	83.43	83.84	84.38	85.08	85.93	86.96

TABLE 2.53.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	91	14	0.722	4.02–2	0.40	–1.08–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
373.0–463.1	644.65	1.94231+1	4.52475	3.97269	2.08442+1		IV



Name: Hydrogen-d_2 peroxide
Formula: D_2O_2

CAS-RN: 6909-54-2
Group No.: 2-054
Molar Mass: 36.03

TABLE 2.54.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
55GIG/MOR2	298.15	2.662	nosp	not specified		C_p	DSTO	55GIG/MOR1

Name: Hydrogen sulfide-d_2
Formula: D_2S

CAS-RN: 13536-94-2
Group No.: 2-055
Molar Mass: 36.09

TABLE 2.55.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38KRU/CLU	N	188.8-202.5	9	nosp	not specified		C_p	BSIO	36CLU/GOL

38KRU/CLU sample contained 0.8 % HDS

TABLE 2.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	9	9	0.688	4.11-2	0.48	3.08-4	-3

Temp. range K	A_1	A_2	Level of uncertainty
188.8-202.5	8.82456	-1.66007-1	IV

TABLE 2.55.4. Recommended values of heat capacities

Temp. (K)	190	195	200
c_p ($J\,K^{-1}g^{-1}$)	1.960	1.958	1.956
C_p ($J\,K^{-1}mol^{-1}$)	70.75	70.68	70.61

Name: Hydrogen selenide-d_2
Formula: D_2Se

CAS-RN: 13536-95-3
Group No.: 2-056
Molar Mass: 82.99

TABLE 2.56.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38KRU/CLU	N	210.9-232.7	12	nosp	not specified		C_p	BSIO	36CLU/GOL

38KRU/CLU sample contained 0.8 % HDSe

TABLE 2.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.748	4.48–2	0.52	3.92–4	2
Temp. range K		A_1	A_2				Level of uncertainty
210.9–232.7		8.90311	–1.52128–1				IV

TABLE 2.56.4. Recommended values of heat capacities

Temp. (K)	210	220	230
c_p (J K^{-1}g^{-1})	0.860	0.858	0.857
C_p (J K^{-1}mol^{-1})	71.37	71.24	71.12

Name: Ammonia–d_3
Formula: D_3N

CAS–RN: 13550–49–7
Group No.: 2–057
Molar Mass: 20.05

TABLE 2.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
72MAN/TOL	N	202.4–216.7	7	1.00	99.99	anal	C_p	BSAO	68BAG/KUC

72MAN/TOL content of heavy isotope 98.2 %

TABLE 2.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.194	1.90–2	0.19	5.24–5	–2
Temp. range K		A_1	A_2				Level of uncertainty
202.4–216.7		6.87015	1.38543				V

TABLE 2.57.4. Recommended values of heat capacities

Temp. (K)	200	205	210	215
c_p (J K^{-1}g^{-1})	4.00	4.03	4.06	4.08
C_p (J K^{-1}mol^{-1})	80.2	80.7	81.3	81.9

Name: Hydrofluoric acid
Formula: FH

CAS–RN: 7664–39–3
Group No.: 2–058
Molar Mass: 20.01

TABLE 2.58.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33DAH/JUN	N	200.0–270.0	8S	nosp	not specified		C_{sat}	BSIO	24EUC/KAR
53HU/WHI1		197.9–289.1	13	nosp	99.8	anal	C_p	BSIO	50JOH/CLA

33DAH/JUN probably the best data for HF (information in 72HOR)

TABLE 2.58.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
53HU/WHI1	197.9–289.1	13	0.50#	0.292	8.15–3	0.15	2.26–5	1
				Rejected data				
33DAH/JUN	(2.12, 27.67, 2.09, 8)							

TABLE 2.58.3. Parameters of regression polynomial

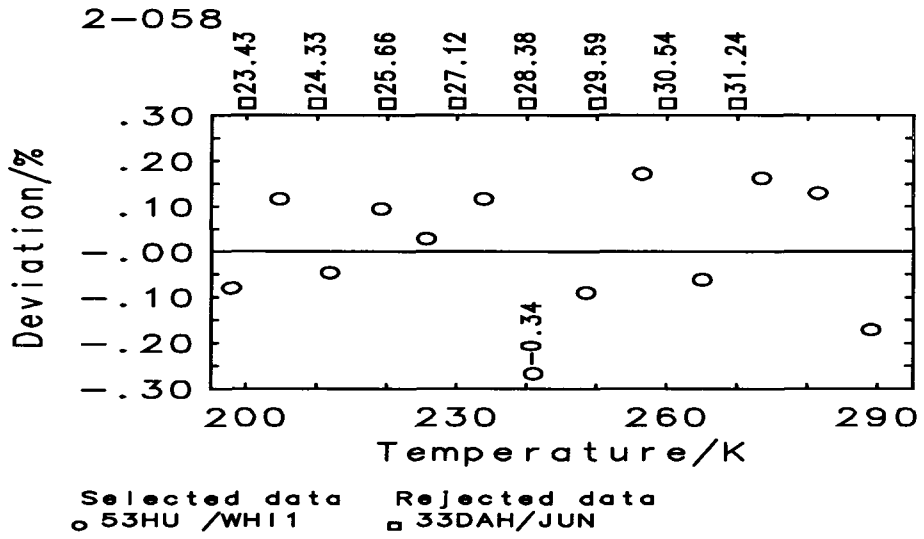
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	13	0.333	9.29–3	0.17	2.26–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
197.9–289.1		7.53087	–2.69185	7.59270–1			III

TABLE 2.58.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1} g^{-1}$)	2.155	2.172	2.196	2.226	2.262	2.305	2.354
C_p ($J K^{-1} mol^{-1}$)	43.10	43.45	43.93	44.53	45.26	46.12	47.10
Temp. (K)	270	273.15	280	290	298.15		
c_p ($J K^{-1} g^{-1}$)	2.410	2.428	2.471	2.539	2.599		
C_p ($J K^{-1} mol^{-1}$)	48.21	48.58	49.44	50.80	52.00		

TABLE 2.58.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	13	0.487	1.38–2	0.24	4.78–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
197.9–289.1	461.00	4.13160	2.54785	2.29853	1.67495		III



Name: Rubidium fluoride ($Rb(HF_2)$)
Formula: F_2HRb

CAS-RN: 12280-64-7
Group No.: 2-059
Molar Mass: 124.47

TABLE 2.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78WES/LAN	492.4–530.2	7	nosp	99.92	melpt	C_p	BSAO	68WES/WES

TABLE 2.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.582	3.33-2	0.23	1.11-4	-1
Temp. range K		A_1	A_2				Level of uncertainty
492.4–530.2		1.06165+1	7.28154-1				III

TABLE 2.59.4. Recommended values of heat capacities

Temp. (K)	490	500	510	520	530
c_p ($J K^{-1} g^{-1}$)	0.947	0.952	0.957	0.962	0.967
C_p ($J K^{-1} mol^{-1}$)	117.9	118.5	119.1	119.8	120.4

Name: Ammonium fluoride ($(NH_4)(HF_2)$)
Formula: F_2H_5N

CAS-RN: 1341-49-7
Group No.: 2-060
Molar Mass: 57.04

TABLE 2.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CAR/WES	406.9–443.5	8	nosp	99.88	melpt	C_p	BSAO	68WES/WES

TABLE 2.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	8	8	0.251	1.73–2	0.10	2.62–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
406.9–443.5		1.17567+1	1.30981				III

TABLE 2.60.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440
c_p ($J K^{-1}g^{-1}$)	2.496	2.515	2.535	2.554
C_p ($J K^{-1}mol^{-1}$)	142.4	143.5	144.6	145.7

Name: Oxygen fluoride
Formula: F_2O

CAS-RN: 7783-41-7
Group No.: 2-061
Molar Mass: 54.00

TABLE 2.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
66FIE	82.0–197.8	26	nosp	99.5	anal	C_{sat}	BSAO	66FIE

TABLE 2.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	26	26	0.971	6.38–2	0.68	8.16–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
82.1–197.9		8.03871	1.01577				IV

TABLE 2.61.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_{sat} (J K^{-1}g^{-1})	1.379	1.394	1.410	1.426	1.441	1.457	1.472
C_{sat} (J K^{-1}mol^{-1})	74.44	75.28	76.13	76.97	77.82	78.66	79.51
Temp. (K)	160	170	180	190	200		
c_{sat} (J K^{-1}g^{-1})	1.488	1.504	1.519	1.535	1.551		
C_{sat} (J K^{-1}mol^{-1})	80.35	81.20	82.04	82.88	83.73		

TABLE 2.61.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	26	26	0.978	6.43–2	0.68	7.77–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
82.1–197.9	215.10	–5.56381–2	3.90601–4	8.10077	1.98130		IV

Name: Thionyl fluoride
Formula: F_2OS

CAS-RN: 7783–42–8
Group No.: 2–062
Molar Mass: 86.06

TABLE 2.62.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
65PAC/TUR	147.0–229.7	39	nosp	99.974	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 2.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	39	39	1.104	4.09–2	0.33	2.51–4	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
147.0–229.7		1.44510+1	–2.31294	6.26343–1			III

TABLE 2.62.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J K^{-1}g^{-1})	1.197	1.194	1.191	1.190	1.190	1.191	1.194
C_{sat} (J K^{-1}mol^{-1})	103.0	102.7	102.5	102.4	102.4	102.5	102.7
Temp. (K)	220	230					
c_{sat} (J K^{-1}g^{-1})	1.197	1.202					
C_{sat} (J K^{-1}mol^{-1})	103.1	103.5					

Name: Sulfuryl fluoride
Formula: F_2O_2S

CAS-RN: 2699-79-8
Group No.: 2-063
Molar Mass: 102.06

TABLE 2.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60BOC/PET	142.3–209.6	20	0.10	99.71	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 2.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	20	20	0.676	8.60–3	0.07	9.92–6	–4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
142.3–209.6	–1.17359+1	4.51180+1	–2.68893+1	5.19590	II

TABLE 2.63.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.058	1.057	1.051	1.041	1.031	1.023	1.019
C_{sat} (J K^{-1}mol^{-1})	108.0	107.9	107.2	106.3	105.2	104.4	104.0

Temp. (K)	210
c_{sat} (J K^{-1}g^{-1})	1.022
C_{sat} (J K^{-1}mol^{-1})	104.3

Name: Nitrogen fluoride (NF_3)
Formula: F_3N

CAS-RN: 7783-54-2
Group No.: 2-064
Molar Mass: 71.00

TABLE 2.64.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55PIE/PAC	70.1–143.8	44	0.10	99.999	melpt	C_{sat}	BSAO	55PAC/PIE
81WEB	67.9–228.9	100	0.60	99.88	melpt	C_{sat}	BSAO	61GOO

TABLE 2.64.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
55PIE/PAC	70.1–143.8	44	0.10	2.998	2.58–2	0.30	5.01–3	4
81WEB	67.9–228.9	100	0.60	1.725	9.68–2	1.03	–7.49–2	–88

TABLE 2.64.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	144	144	2.241	8.37–2	0.90	–5.05–2	–84
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
67.9–150.0		1.12335+1	–5.62316	3.12811	–3.10740–1		III
150.0–210.0		–9.04221	3.49283+1	–2.39062+1	5.69688		IV
210.0–228.9		–7.08988+3	1.01504+4	–4.84080+3	7.70284+2		V

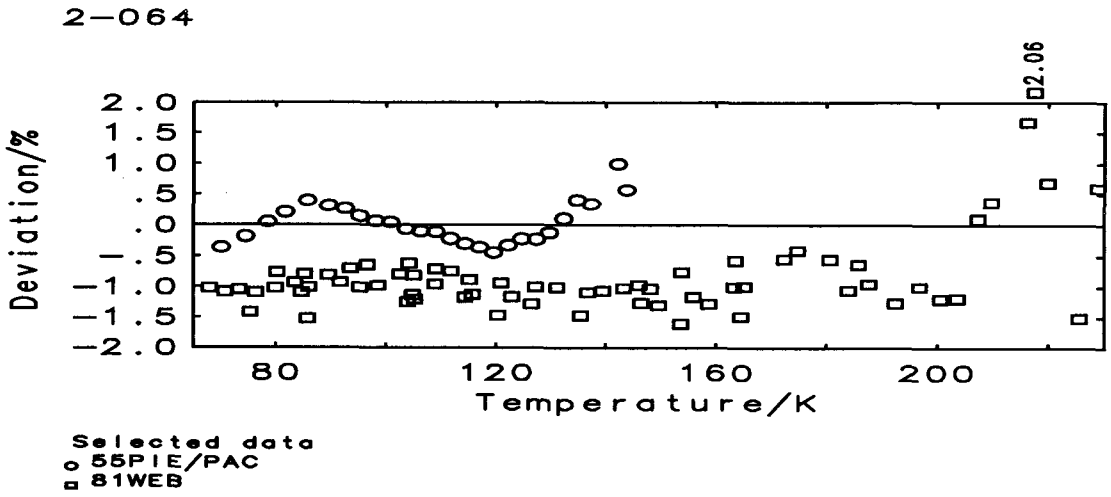
TABLE 2.64.4. Recommended values of heat capacities

Temp. (K)	70	80	90	100	110	120	130
c_{sat} (J K^{-1}g^{-1})	1.022	1.004	0.993	0.987	0.986	0.990	0.999
C_{sat} (J K^{-1}mol^{-1})	72.53	71.32	70.51	70.07	70.00	70.28	70.90
Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.012	1.029	1.051	1.082	1.124	1.182	1.261
C_{sat} (J K^{-1}mol^{-1})	71.83	73.07	74.64	76.79	79.79	83.94	89.50
Temp. (K)	210	220	230				
c_{sat} (J K^{-1}g^{-1})	1.36	1.58	2.37				
C_{sat} (J K^{-1}mol^{-1})	96.8	112	168				

TABLE 2.64.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	144	73	4.742	5.08–2	0.56	9.92–3	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
111.8–228.9	234.00	–1.86809	1.23546–1	7.88781	8.10292–1	–9.48440	7.30941	IV



Name: Phosphoryl fluoride
Formula: F_3OP

CAS-RN: 13478-20-1
Group No.: 2-065
Molar Mass: 103.97

TABLE 2.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70PAC/JEP	235.3–241.2	4	nosp	99.926	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 2.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	4	4	0.661	2.09–2	0.13	2.77–5	–2
Temp. range K		A_1	A_2				Level of uncertainty
235.3–241.2		1.61491+1	–1.62846–1				II

TABLE 2.65.4. Recommended values of heat capacities

Temp. (K)	235	237	239	241
c_{sat} (J $K^{-1}g^{-1}$)	1.261	1.261	1.260	1.260
C_{sat} (J $K^{-1}mol^{-1}$)	131.1	131.1	131.0	131.0

Name: Phosphorous trifluoride
Formula: F_3P

CAS-RN: 7783-55-3
Group No.: 2-066
Molar Mass: 87.97

TABLE 2.66.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62PAC/PET	123.4–168.7	18	nosp	99.69	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 2.66.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	18	18	0.841	1.93–2	0.17	5.47–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
123.4–168.7		1.48344+1	–4.51807	1.50975			II

TABLE 2.66.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170
c_{sat} (J $K^{-1}g^{-1}$)	1.088	1.084	1.083	1.084	1.089
C_{sat} (J $K^{-1}mol^{-1}$)	95.72	95.35	95.24	95.37	95.76

Name: Iodine fluoride (IF_5)
Formula: F_5I

CAS-RN: 7783-66-6
Group No.: 2-067
Molar Mass: 221.90

TABLE 2.67.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71OSB/SCH	288.2–345.5	7	0.10	99.985	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 2.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	7	7	0.135	2.83–3	0.01	2.72–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
288.2–345.5		2.74430+1	−3.83116	5.60825−1			II

TABLE 2.67.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J $K^{-1}g^{-1}$)	0.789	0.787	0.787	0.785	0.784	0.783	0.783
C_{sat} (J $K^{-1}mol^{-1}$)	175.0	174.7	174.6	174.2	174.0	173.8	173.8
Temp. (K)	350						
c_{sat} (J $K^{-1}g^{-1}$)	0.783						
C_{sat} (J $K^{-1}mol^{-1}$)	173.8						

Name: Niobium fluoride (NbF_5)
Formula: F_5Nb

CAS-RN: 7783-68-8
Group No.: 2-068
Molar Mass: 187.90

TABLE 2.68.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60BRA/MYE	N	375.0–475.0	3S	nosp	99.1	anal	C_{avg}	DSIO	62BRA/MYE

60BRA/MYE values calculated from temperature dependence of enthalpy by the compilers

TABLE 2.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	3	3	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
375.0–475.0		−5.16983	8.62509	−7.34692−1			V

TABLE 2.68.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c ($J K^{-1}g^{-1}$)	0.75	0.77	0.78	0.79	0.80	0.81	0.82
C ($J K^{-1}mol^{-1}$)	141	144	146	148	150	152	154
Temp. (K)	450	460	470				
c ($J K^{-1}g^{-1}$)	0.83	0.84	0.85				
C ($J K^{-1}mol^{-1}$)	156	158	159				

Name: Molybdenum fluoride (MoF_6)
Formula: F_6Mo

CAS-RN: 7783-77-9
Group No.: 2-069
Molar Mass: 209.93

TABLE 2.69.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Method	Type capacity	Calorimeter Type	Reference
60BRA/MYE	298.15	0.7894	nosp	99.98	melpt	C_p	BSIO	36PEA/BAK

Name: Sulfur fluoride (SF_6)
Formula: F_6S

CAS-RN: 2551-62-4
Group No.: 2-070
Molar Mass: 146.06

TABLE 2.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38EUC/SCH	225.0-230.0	2	nosp	99.6	melpt	C_p	BSAO	38EUC/SCH

TABLE 2.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	1.91-6	0
Temp. range K		A_1	A_2				Level of uncertainty
225.0-230.0		-3.33130+1	2.07326+1				IV

TABLE 2.70.4. Recommended values of heat capacities

Temp. (K)	225	230
c_p ($J K^{-1}g^{-1}$)	0.759	0.818
C_p ($J K^{-1}mol^{-1}$)	110.9	119.5

Name: Uranium(VI) fluoride
Formula: F_6U

CAS-RN: 7783-81-5
Group No.: 2-071
Molar Mass: 352.02

TABLE 2.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48BRI/HOG	337.2–370.0	8S	1.00	99.98	melpt	C_{sat}	BSAO	45SCO/MEY
53LLE	343.1–373.1	4S	1.00	not specified		C_{sat}	BSIO	53LLE

TABLE 2.71.2. Correlated heat capacities

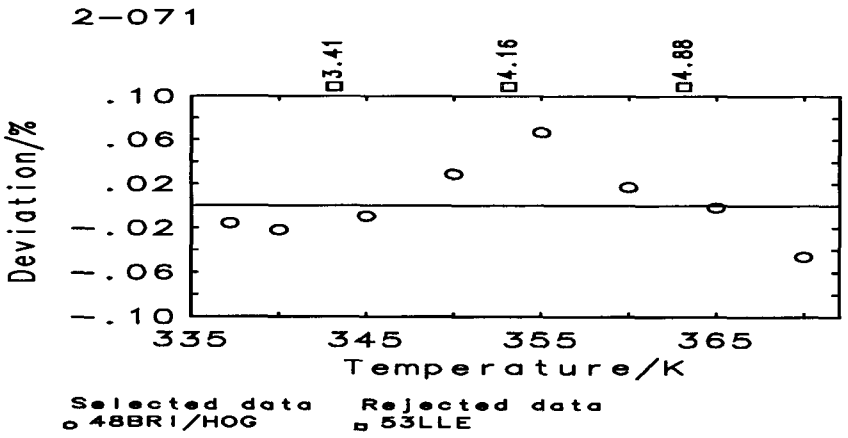
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48BRI/HOG	337.2–370.0	8	1.00	0.033	7.58–3	0.03	5.01–6	–1
				Rejected data				
53LLE	(1.02, 4.19, 1.01, 3)							

TABLE 2.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	8	0.038	8.75–3	0.04	5.01–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
337.2–370.0		1.75393+1	1.60265				IV

TABLE 2.71.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	0.543	0.547	0.551	0.554
C_{sat} (J K^{-1}mol^{-1})	191.1	192.5	193.8	195.1



Name: Germane
Formula: GeH_4

CAS-RN: 7782-65-2
Group No.: 2-072
Molar Mass: 76.64

TABLE 2.72.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
42CLU/FAB	112.7–165.4	8	nosp	not specified		C_p	BSIO	36CLU/GOL

TABLE 2.72.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	1.089	6.43–2	0.87	6.97–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
112.7–165.4		1.21719+1	–7.34650	2.75449			IV

TABLE 2.72.4. Recommended values of heat capacities

Temp. (K)	110	120	130	140	150	160	170
c_p ($J K^{-1} g^{-1}$)	0.805	0.794	0.789	0.790	0.797	0.810	0.829
C_p ($J K^{-1} mol^{-1}$)	61.72	60.88	60.50	60.58	61.11	62.10	63.55

Name: Hydroiodic acid
Formula: HI

CAS-RN: 10034-85-2
Group No.: 2-073
Molar Mass: 127.91

TABLE 2.73.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24EUC/KAR	224.0–238.0	3	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
29GIA/WIE	227.1–236.1	3	nosp	not specified		C_{sat}	BSIO	28GIA/WIE1

TABLE 2.73.2. Correlated heat capacities

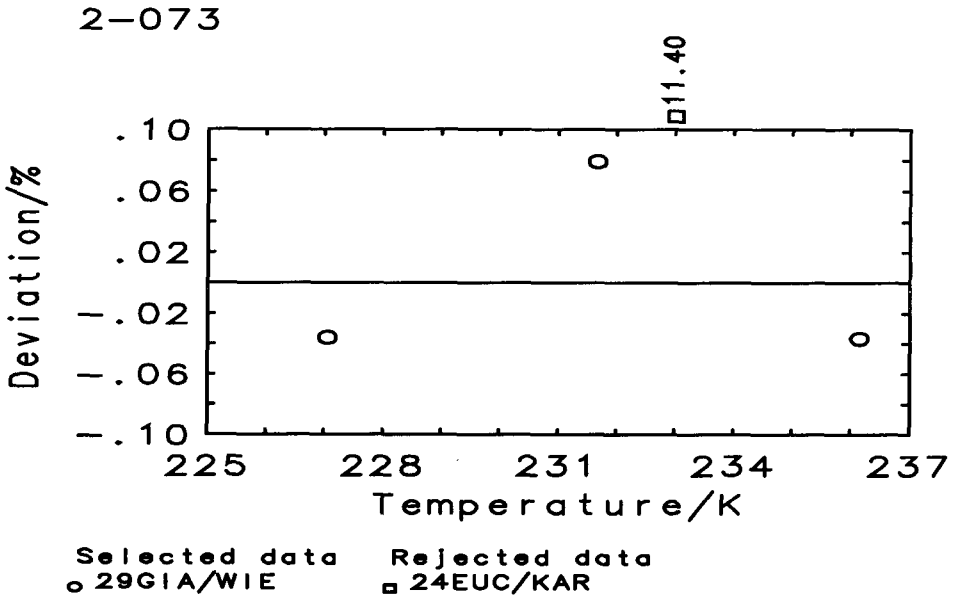
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
29GIA/WIE	227.1–236.1	3	0.50#	0.109	3.90–3	0.05	4.45–6	–1
				Rejected data				
24EUC/KAR	(9.20–1, 11.39, 9.20–1, 1)							

TABLE 2.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_{sat}	6	3	0.189	6.76–3	0.09	4.45–6	−1
Temp. range K		A_1	A_2				Level of uncertainty
227.1–236.1		9.60416	−1.05055				IV

TABLE 2.73.4. Recommended values of heat capacities

Temp. (K)	230	232	234	236
c_{sat} (J K^{-1}g^{-1})	0.467	0.466	0.464	0.463
C_{sat} (J K^{-1}mol^{-1})	59.76	59.59	59.41	59.24



Name: Nitric acid
Formula: HNO_3

CAS-RN: 7697–37–2
Group No.: 2–074
Molar Mass: 63.01

TABLE 2.74.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
42FOR/GIA	236.6–302.9	10	0.10	99.99	melpt	C_p	BSIO	37GIA/EGA

TABLE 2.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.576	3.06–2	0.23	1.12–4	2
Temp. range K		A_1	A_2				Level of uncertainty
236.6–302.9		1.42869+1	–3.55116–1				III

TABLE 2.74.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.773	1.768	1.763	1.759	1.757	1.754	1.749
C_p (J K^{-1}mol^{-1})	111.7	111.4	111.1	110.8	110.7	110.5	110.2
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.745	1.745					
C_p (J K^{-1}mol^{-1})	110.0	109.9					

Name: Water
Formula: H_2O

CAS–RN: 7732–18–5
Group No.: 2–075
Molar Mass: 18.02

TABLE 2.75.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
05DIE	N	287.7–576.4	20	nosp	not specified		C_{avg}	DSTO	05DIE
21JAE/VON		277.9–322.8	67	nosp	not specified		C_p	BSIO	21JAE/VON
37OSB/STI	N	375.6–647.2	63S	nosp	not specified		C_{sat}	BSAO	37OSB/STI
39OSB/STI	N	273.6–368.1	20S	nosp	not specified		C_p	BSAO	39OSB/STI
40COC/FER	N	290.0–321.2	25	nosp	not specified		C_{sat}	BDHO	40COC/FER
56SCH/GOT		277.0–293.1	19	2.00	not specified		C_p	BSAO	33SOU/BRI
59COX/SMI		276.9–295.3	3	nosp	not specified		C_p	BSAO	59COX/SMI
70KRE		298.1	1	nosp	not specified		C_p	BSAO	63BEN
78BYV/JAS		293.1–333.1	3	2.00	not specified		C_p	BDCT	78BYV/JAS
86NAZ/BAS1		318.6–364.1	3	2.00	not specified		C_p	BDHO	86NAZ/BAS1

05DIE average values between the given temperatures and 273.15 K
37OSB/STI values calculated from temperature dependence of enthalpy by the compiler
39OSB/STI same data in 53GIN/FUR
40COC/FER preliminary data published in 36FER/COC

TABLE 2.75.2. Correlated heat capacities

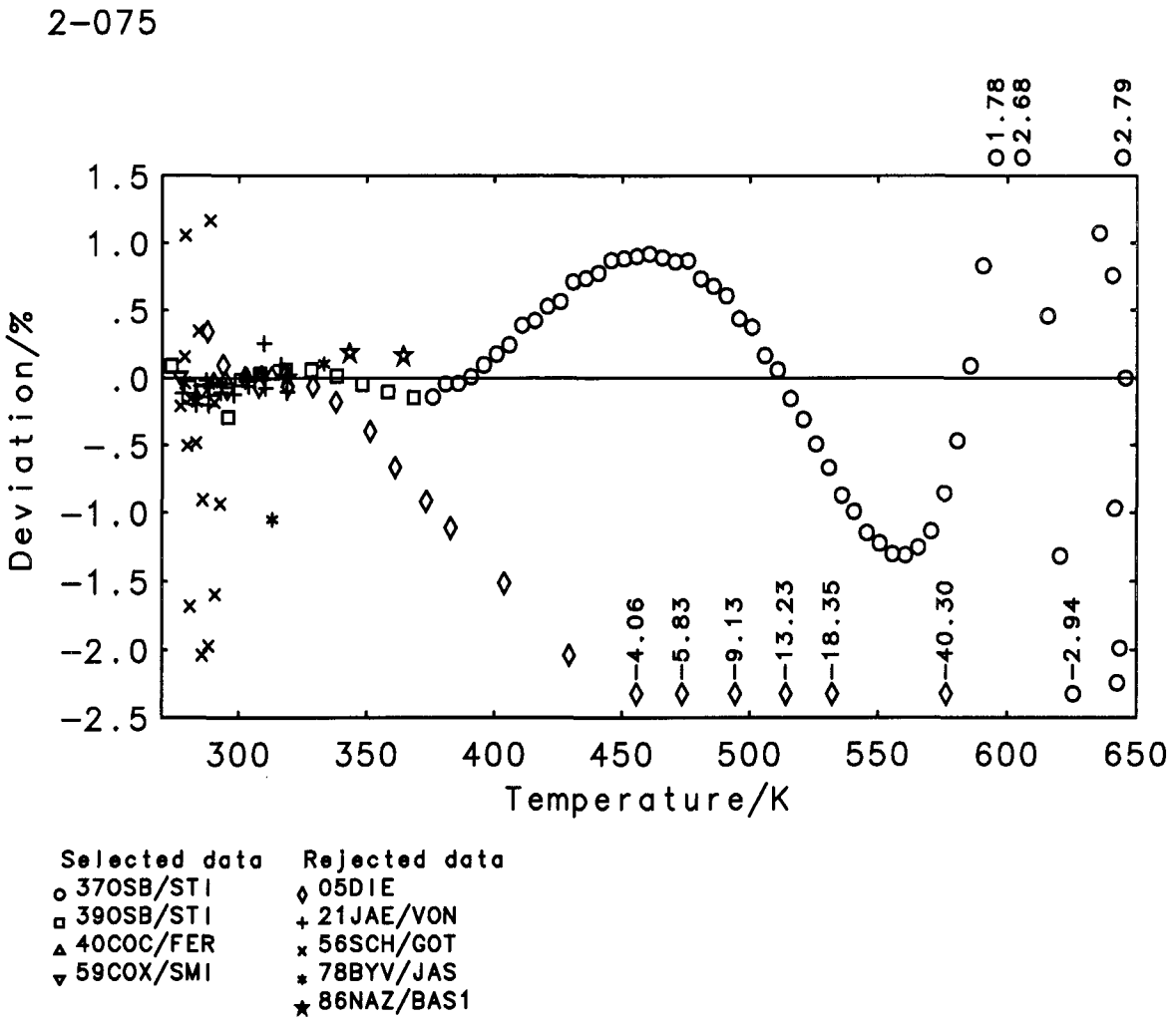
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
37OSB/STI	375.6–644.7	60	1.00#	2.609	1.98	2.61	1.32–1	13
39OSB/STI	273.6–368.1	20	0.10#	0.893	8.10–3	0.09	–2.51–3	–2
40COC/FER	290.0–321.2	25	0.10#	0.250	2.27–3	0.03	1.76–3	18
59COX/SMI	277.0–295.3	3	0.20#	0.353	6.40–3	0.07	–5.00–3	–2
70KRE	298.1	1	0.20#	0.095	1.73–3	0.02	–1.73–3	–1

TABLE 2.75.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	112	109	2.045	1.52	2.00	7.23–2	26
C_{sat}	224	109	1.054	2.48–1	0.96	1.16–2	21
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
273.6–380.0		2.09634+1	−1.01344+1	2.82530	−2.56738−1		II
380.0–590.0		−2.20666+1	2.38366+1	−6.11445	5.27450−1		IV
590.0–635.0		−4.01518+4	2.04288+4	−3.46458+3	1.95921+2		V
635.0–644.6		−2.38034+7	1.12472+7	−1.77145+6	9.30037+4		V
273.6–380.0		1.91935+1	−8.46779	2.30596	−2.03214−1		II
380.0–590.0		−1.20682+1	1.62126+1	−4.18887	3.66508−1		IV
590.0–635.0		−1.75899+4	8.95411+3	−1.51909+3	8.59539+1		V
635.0–644.6		−5.92160+6	2.79825+6	−4.40779+5	2.31442+4		V

TABLE 2.75.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	4.201	4.187	4.181	4.180	4.177	4.178	4.182
C_p (J K^{-1}mol^{-1})	75.67	75.44	75.31	75.30	75.24	75.26	75.34
c_{sat} (J K^{-1}g^{-1})	4.201	4.188	4.181	4.180	4.177	4.177	4.181
C_{sat} (J K^{-1}mol^{-1})	75.67	75.45	75.32	75.30	75.24	75.25	75.32
Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	4.189	4.198	4.208	4.218	4.229	4.238	4.249
C_p (J K^{-1}mol^{-1})	75.46	75.62	75.80	75.99	76.18	76.36	76.54
c_{sat} (J K^{-1}g^{-1})	4.187	4.196	4.206	4.217	4.229	4.241	4.254
C_{sat} (J K^{-1}mol^{-1})	75.44	75.59	75.78	75.98	76.19	76.40	76.63
Temp. (K)	410	420	430	440	450	460	470
c_p (J K^{-1}g^{-1})	4.261	4.277	4.297	4.324	4.359	4.403	4.458
C_p (J K^{-1}mol^{-1})	76.76	77.04	77.41	77.90	78.53	79.32	80.31
c_{sat} (J K^{-1}g^{-1})	4.268	4.286	4.308	4.334	4.367	4.406	4.454
C_{sat} (J K^{-1}mol^{-1})	76.90	77.21	77.60	78.08	78.67	79.38	80.24
Temp. (K)	480	490	500	510	520	530	540
c_p (J K^{-1}g^{-1})	4.525	4.606	4.701	4.814	4.944	5.094	5.265
C_p (J K^{-1}mol^{-1})	81.52	82.97	84.70	86.72	89.07	91.78	94.86
c_{sat} (J K^{-1}g^{-1})	4.511	4.577	4.655	4.745	4.848	4.965	5.097
C_{sat} (J K^{-1}mol^{-1})	81.26	82.46	83.86	85.48	87.34	89.44	91.83
Temp. (K)	550	560	570	580	590	600	610
c_p (J K^{-1}g^{-1})	5.459	5.676	5.919	6.188	6.486	6.90	7.89
C_p (J K^{-1}mol^{-1})	98.34	102.3	106.6	111.5	116.8	124	142
c_{sat} (J K^{-1}g^{-1})	5.245	5.411	5.594	5.797	6.020	6.30	6.85
C_{sat} (J K^{-1}mol^{-1})	94.50	97.48	100.8	104.4	108.5	114	123
Temp. (K)	620	630	640				
c_p (J K^{-1}g^{-1})	10.0	13.8	25.1				
C_p (J K^{-1}mol^{-1})	180	248	452				
c_{sat} (J K^{-1}g^{-1})	7.89	9.66	13.7				
C_{sat} (J K^{-1}mol^{-1})	142	174	248				



Name: Hydrogen peroxide
Formula: H_2O_2

CAS-RN: 7722-84-1
Group No.: 2-076
Molar Mass: 34.01

TABLE 2.76.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
20MAA/HAT	N	282.4	1	2.00	not specified		C_{avg}	DSIO	20MAA/HAT
51FOL/GIG	N	285.6	1	0.25	99.8	anal	C_{avg}	DSTO	51FOL/GIG
55GIG/MOR2		298.1	1	nosp	not specified		C_p	DSTO	55GIG/MOR1
62GIG/CAR	N	309.1-316.6	2S	nosp	not specified		C_{avg}	DSTO	55GIG/MOR1
64KRO/VEN	N	293.1-333.1	3S	nosp	not specified		C_p	BSIO	64KRO/VEN

20MAA/HAT average value in temperature range 273-292 K
51FOL/GIG average value in temperature range 273-298 K
62GIG/CAR extrapolated data obtained from measurement with aqueous solutions (max. concentration 90 mass %)
64KRO/VEN extrapolated data obtained from measurement with aqueous solutions (max. concentration 80 mass %)

TABLE 2.76.2. Correlated heat capacities

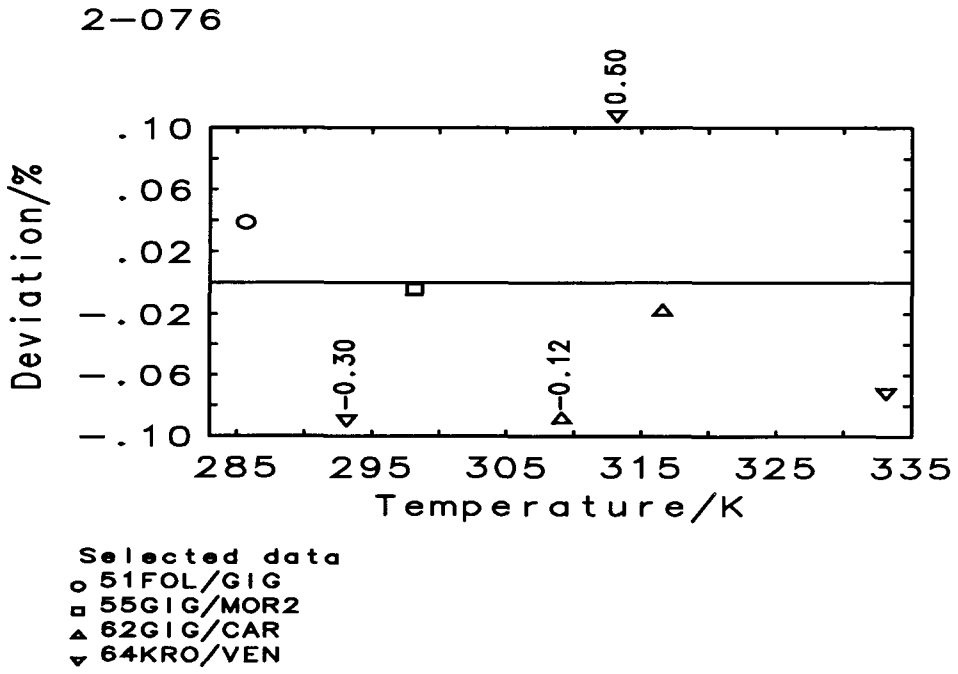
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
51FOL/GIG	285.6	1	0.25	0.146	3.93–3	0.04	3.93–3	1
55GIG/MOR2	298.1	1	0.40#	0.016	6.83–4	0.01	–6.83–4	0
62GIG/CAR	309.1–316.6	2	0.40#	0.218	9.35–3	0.09	–7.63–3	–2
64KRO/VEN	293.1–333.1	3	0.60#	0.567	3.67–2	0.34	4.69–3	–1

TABLE 2.76.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.520	3.25–2	0.30	2.94–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
285.6–333.1		3.00483+1	–1.26522+1	2.07198			IV

TABLE 2.76.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.656	2.636	2.626	2.625	2.625	2.635	2.655
C_p (J K^{-1}mol^{-1})	90.35	89.65	89.33	89.29	89.28	89.62	90.30



Name: Sulfuric acid
Formula: H_2O_4S

CAS–RN: 7664–93–9
Group No.: 2–077
Molar Mass: 98.08

TABLE 2.77.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*90PIC		284.0–334.0	eqn	4.00	not specified		C_p	BDHO	*90PIC
32SOC	N	295.6–353.1	4S	nosp	not specified		C_p	not specified	
52RUB/GIA		287.7–305.7	4	0.20	99.94	melpt	C_p	BSIO	37GIA/EGA

32SOC values at 295.65 K and 313.15 K are unpublished data by Savarizky

TABLE 2.77.2. Correlated heat capacities

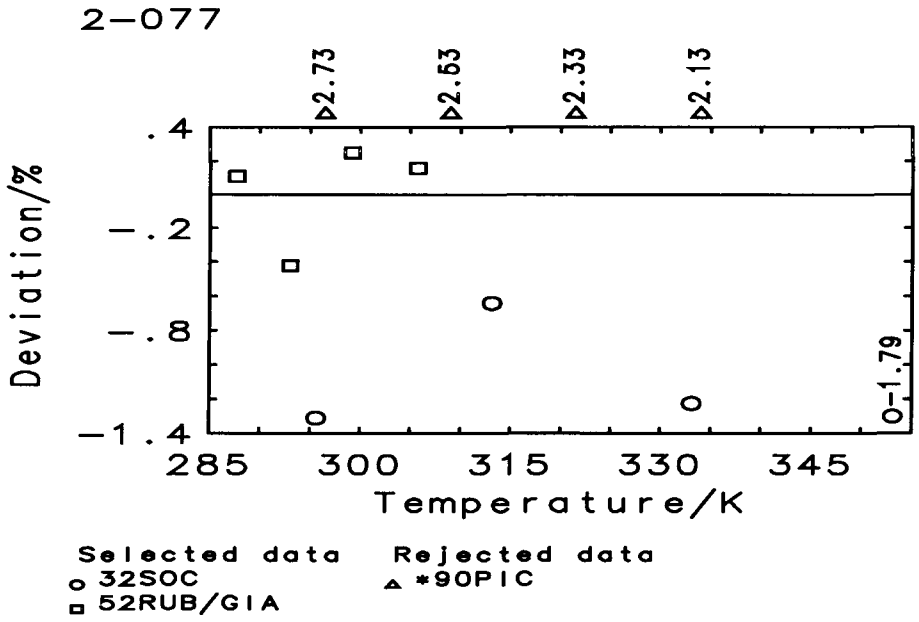
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
32SOC	295.6–353.1	4	1.50#	0.872	2.26–1	1.31	–2.13–1	–4
52RUB/GIA	287.7–305.7	4	0.20	1.321	4.38–2	0.26	4.12–3	2
				Rejected data				
*90PIC	(4.26–1, 2.44, 4.24–1, 4)							

TABLE 2.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	8	1.293	1.88–1	1.09	–1.05–1	–2
Temp. range K		A_1	A_2				Level of uncertainty
287.7–353.1		9.22774	2.49400				IV

TABLE 2.77.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.395	1.413	1.417	1.438	1.459	1.480	1.501
C_p (J K^{-1}mol^{-1})	136.9	138.5	138.9	141.0	143.1	145.2	147.2
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	1.522						
C_p (J K^{-1}mol^{-1})	149.3						



Name: Disulfuric acid
Formula: $H_2O_7S_2$

CAS-RN: 7783-05-3
Group No.: 2-078
Molar Mass: 178.14

TABLE 2.78.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity Method	Type capacity	Calorimeter Type	Calorimeter Reference
26AUE	308.15	1.351	nosp	not specified		C_{avg}	DSIO	26AUE

Name: Hydrogen sulfide
Formula: H_2S

CAS-RN: 7783-06-4
Group No.: 2-079
Molar Mass: 34.08

TABLE 2.79.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36CLU/FRA2	193.6-208.9	4	nosp	not specified		C_p	BSIO	36CLU/GOL
36GIA/BLU	189.9-211.0	6	nosp	99.999	melpt	C_p	BSIO	28GIA/WIE1

TABLE 2.79.2. Correlated heat capacities

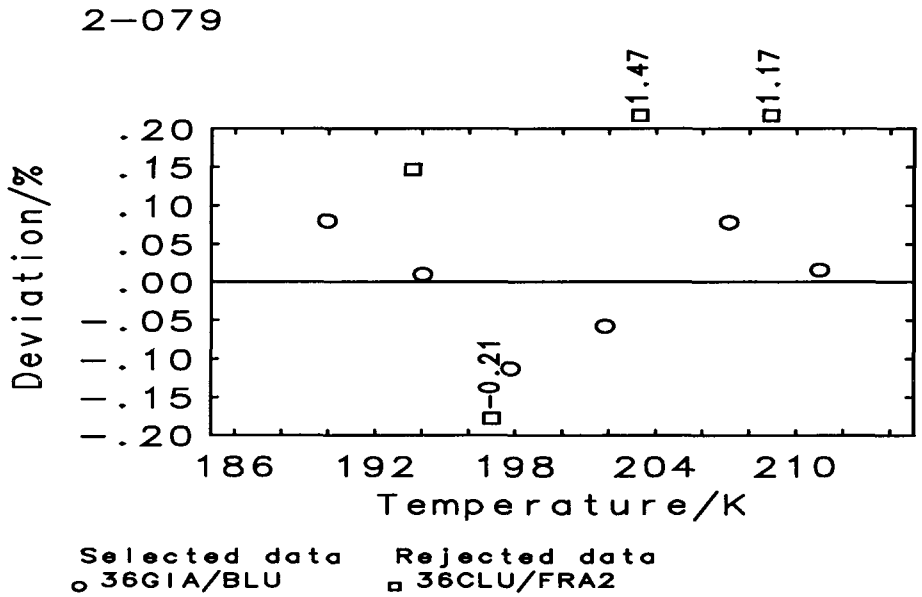
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
36GIA/BLU	189.9–211.0	6	0.30#	0.231	5.67–3	0.07	8.11–6	1
				Rejected data				
36CLU/FRA2	(7.87–2, 0.95, 5.34–2, 2)							

TABLE 2.79.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	6	0.283	6.94–3	0.08	8.11–6	1
Temp. range K		A_1	A_2				Level of uncertainty
189.9–211.0	7.	64899	2.64168–1				II

TABLE 2.79.4. Recommended values of heat capacities

Temp. (K)	190	195	200	205	210
c_p (J K^{-1}g^{-1})	1.988	1.992	1.995	1.998	2.001
C_p (J K^{-1}mol^{-1})	67.77	67.88	67.99	68.10	68.21



Name: Hydrogen sulfide (H_2S_2)
Formula: H_2S_2

CAS–RN: 13465–07–1
Group No.: 2–080
Molar Mass: 66.15

TABLE 2.80.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30BUT/MAA	N	184.1–298.1	2	5.00	not specified		C_{avg}	DSIO	20MAA/HAT
63FEH/SEY		239.8–313.1	5	2.00	not specified		C_p	BSAO	63FEH/SEY

30BUT/MAA constant value calculated from temperature dependence of enthalpy by the authors

TABLE 2.80.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
63FEH/SEY	239.8–313.1	5	2.00	0.252	5.63–2	0.50	5.73–4	–1
				Rejected data				
30BUT/MAA	(1.16–1, 1.05, –1.16–1, –1)							

TABLE 2.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	5	0.325	7.27–2	0.65	5.73–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
239.8–313.1		9.74820	4.87109–1				V

TABLE 2.80.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.37	1.38	1.38	1.39	1.39	1.40	1.40
C_p (J K^{-1}mol^{-1})	90.8	91.2	91.6	92.0	92.1	92.4	92.8
Temp. (K)	298.15	300	310				
c_p (J K^{-1}g^{-1})	1.41	1.41	1.42				
C_p (J K^{-1}mol^{-1})	93.1	93.2	93.6				

Name: Hydrogen sulfide (H_2S_3)
Formula: H_2S_3

CAS–RN: 13845–23–3
Group No.: 2–081
Molar Mass: 98.21

TABLE 2.81.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63FEH/SEY	236.9–295.9	5	2.00	not specified		C_p	BSAO	63FEH/SEY

TABLE 2.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.312	9.19–2	0.62	6.84–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
236.9–296.0		1.32735+1	5.23184–1				V

TABLE 2.81.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.23	1.23	1.24	1.24	1.24	1.25	1.25
C_p (J K^{-1}mol^{-1})	121	121	122	122	122	123	123
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.26	1.26					
C_p (J K^{-1}mol^{-1})	123	123					

Name: Hydrogen sulfide (H_2S_4)
Formula: H_2S_4

CAS–RN: 13845–25–5
Group No.: 2–082
Molar Mass: 130.28

TABLE 2.82.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63FEH/SEY	245.8–293.1	5	2.00	not specified		C_p	BSAO	63FEH/SEY

TABLE 2.82.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.171	6.28–2	0.34	2.59–4	1
Temp. range K		A_1	A_2				Level of uncertainty
245.8–293.1		1.64246+1	7.33620–1				V

TABLE 2.82.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.17	1.17	1.17	1.18	1.18	1.18	1.19
C_p (J K^{-1}mol^{-1})	152	152	153	153	154	154	155

Name: Hydrogen sulfide (H_2S_5)
Formula: H_2S_5

CAS–RN: 13845–24–4
Group No.: 2–083
Molar Mass: 162.35

TABLE 2.83.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63FEH/SEY	244.1–293.1	5	2.00	not specified		C_p	BSAO	63FEH/SEY

TABLE 2.83.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.405	1.79–1	0.81	1.75–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
244.1–293.1		1.86800+1	1.26655				V

TABLE 2.83.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	1.12	1.13	1.13	1.13	1.14	1.14	1.15
C_p ($J K^{-1} mol^{-1}$)	182	183	184	184	185	186	187

Name: Hydrogen sulfide (H_2S_6)
Formula: H_2S_6

CAS–RN: 13845–51–7
Group No.: 2–084
Molar Mass: 194.41

TABLE 2.84.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63FEH/SEY	246.8–312.9	5	2.00	not specified		C_p	BSAO	63FEH/SEY

TABLE 2.84.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.807	4.16–1	1.62	8.05–3	0
Temp. range K		A_1	A_2				Level of uncertainty
246.8–313.0		2.05033+1	1.84926				V

TABLE 2.84.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J\,K^{-1}g^{-1}$)	1.07	1.08	1.09	1.09	1.10	1.11	1.11
C_p ($J\,K^{-1}mol^{-1}$)	209	210	212	212	214	215	216

Temp. (K)	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.11	1.12
C_p ($J\,K^{-1}mol^{-1}$)	217	218

Name: Hydrogen selenide
Formula: H_2Se

CAS-RN: 7783-07-5
Group No.: 2-085
Molar Mass: 80.98

TABLE 2.85.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38KRU/CLU	210.4–229.7	10	nosp	not specified		C_p	BSIO	36CLU/GOL

TABLE 2.85.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.411	2.70-2	0.33	1.42-4	-2

Temp. range K	A_1	A_2	Level of uncertainty
210.4–229.7	8.93420	-3.44971-1	IV

TABLE 2.85.4. Recommended values of heat capacities

Temp. (K)	210	220	230
c_p ($J\,K^{-1}g^{-1}$)	0.843	0.839	0.836
C_p ($J\,K^{-1}mol^{-1}$)	68.26	67.97	67.69

Name: Ammonia
Formula: H_3N

CAS-RN: 7664-41-7
Group No.: 2-086
Molar Mass: 17.03

TABLE 2.86.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24EUC/KAR	199.5–221.1	7	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
26DAN/JEN	246.8–290.4	10	2.00	not specified		C_{sat}	BSIO	26DAN/JEN
37OVE/GIA	197.8–238.3	13	nosp	99.999	melpt	C_{sat}	BSIO	37GIA/EGA
71POP/MAN	199.2–200.8	2	1.00	99.99	anal	C_p	BSAO	68BAG/KUC

TABLE 2.86.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
26DAN/JEN	246.9–290.4	10	2.00	1.025	1.99–1	2.05	9.62–2	4
37OVE/GIA	197.8–238.3	13	0.30#	0.750	2.03–2	0.22	–1.46–3	–1
71POP/MAN	199.2–200.8	2	1.00	0.095	8.43–3	0.10	2.20–3	0
				Rejected data				
24EUC/KAR	(3.34–1, 3.61, 3.13–1, 7)							

TABLE 2.86.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	25	0.900	1.35–1	1.39	3.79–2	3
C_{sat}	32	25	0.894	1.35–1	1.40	3.78–2	3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
197.8–290.4	1.01781+1	–1.87331	6.06344–1	V
197.8–290.4	9.89140	–1.59465	5.38618–1	V

TABLE 2.86.4. Recommended values of heat capacities

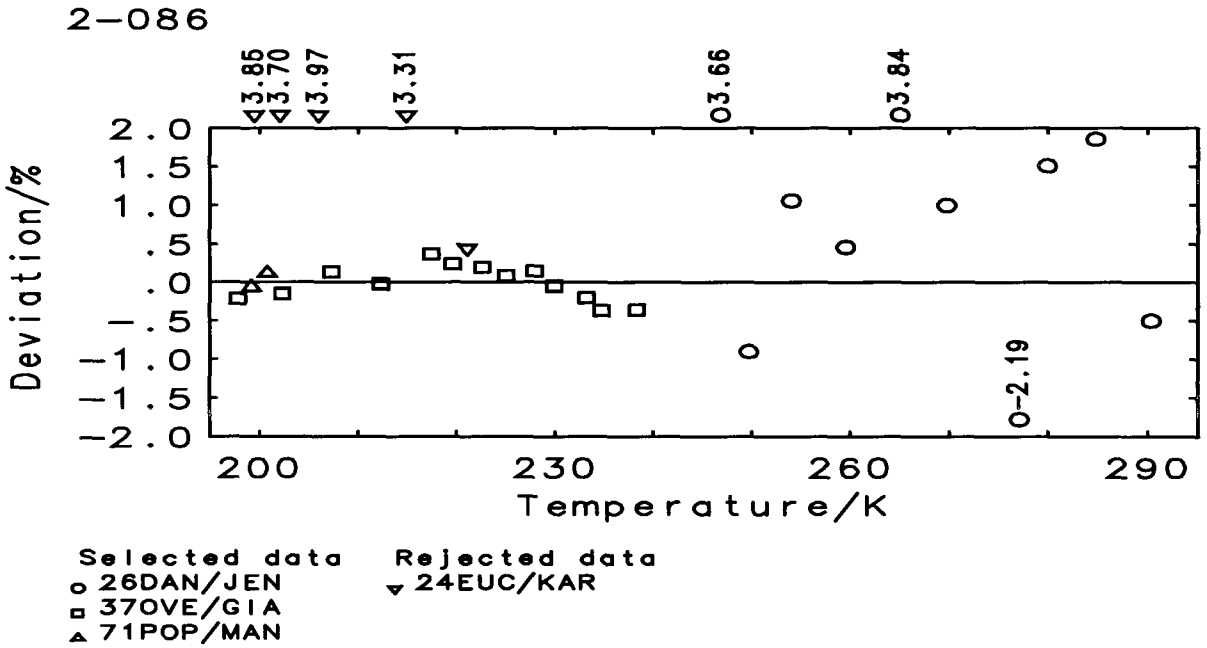
Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	4.32	4.35	4.39	4.43	4.48	4.53	4.59
C_p ($J K^{-1}mol^{-1}$)	73.6	74.1	74.8	75.5	76.3	77.2	78.2
c_{sat} ($J K^{-1}g^{-1}$)	4.32	4.35	4.39	4.43	4.48	4.53	4.58
C_{sat} ($J K^{-1}mol^{-1}$)	73.6	74.1	74.7	75.4	76.2	77.1	78.0

Temp. (K)	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	4.66	4.68	4.73	4.81	4.87
C_p ($J K^{-1}mol^{-1}$)	79.3	79.7	80.5	81.9	83.0
c_{sat} ($J K^{-1}g^{-1}$)	4.64	4.66	4.71	4.78	4.85
C_{sat} ($J K^{-1}mol^{-1}$)	79.1	79.4	80.2	81.5	82.5

TABLE 2.86.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	23	5.286	1.85–1	2.02	6.89–2	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
197.8–290.4	405.60	5.03149	3.84393–1	3.05052	1.64648+1	V



Name: Phosphoric acid
Formula: H_3O_4P

CAS-RN: 7664-38-2
Group No.: 2-087
Molar Mass: 98.00

TABLE 2.87.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
58EGA/LUF	N	288.1–353.1	6S	nosp	not specified	C_p	BSAO	45SCO/MEY
69SMI/MAT	N	335.6	1	nosp	not specified	C_{avg}	DSIO	69SMI/MAT
72WAK/LUF	N	323.1–473.1	16S	nosp	not specified	C_p	DSIO	50EGA/WAK
81LUF	N	300.0–530.0	24S	nosp	not specified	C_{sat}	BDHT	69PER/COM

58EGA/LUF extrapolated data obtained from measurement in aqueous solutions (max. concentration 85 mass %)
69SMI/MAT average value in temperature range 298–373 K; interpolated from data in aqueous solution of P_2O_5
72WAK/LUF interpolated by the compilers from C_p of solutions of P_2O_5 in H_3PO_4 (concentration range of P_2O_5: 72.3 to 84.8 mass %)
81LUF interpolated from measurements in aqueous solutions of P_2O_5

TABLE 2.87.2. Correlated heat capacities

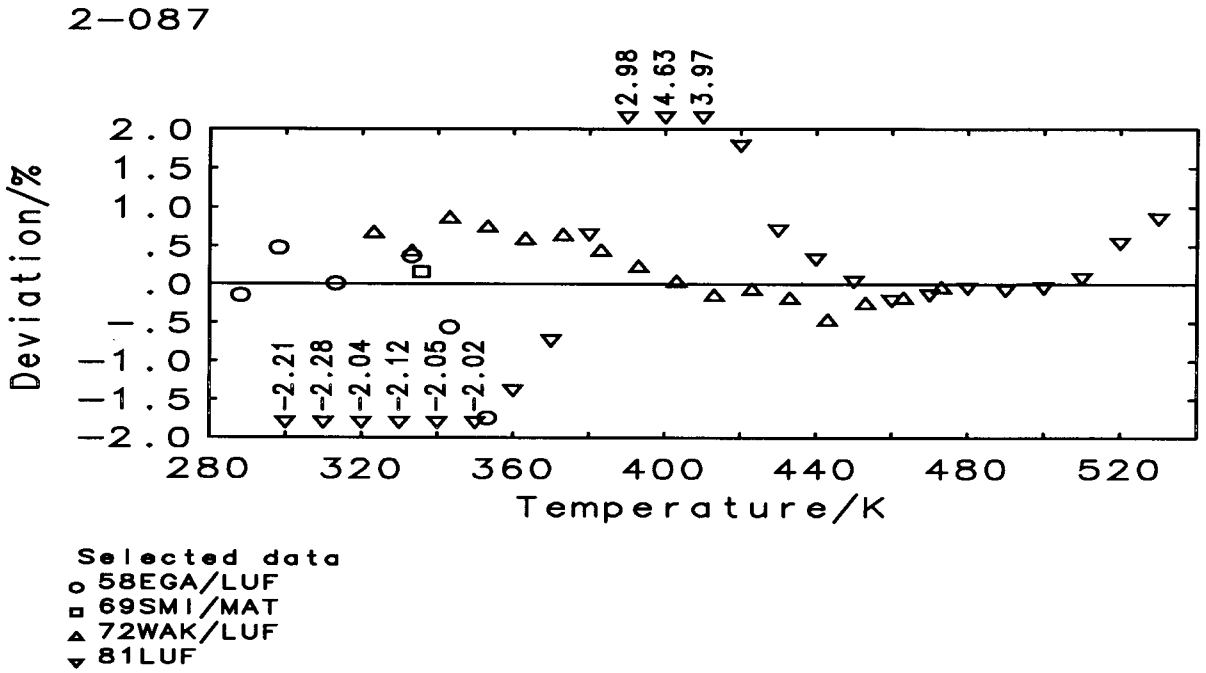
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
58EGA/LUF	288.1–353.1	6	0.50#	1.578	1.56–1	0.79	–5.30–2	–1
69SMI/MAT	335.6	1	1.00#	0.160	3.16–2	0.16	3.16–2	1
72WAK/LUF	323.1–473.1	16	0.70#	0.641	9.19–2	0.45	3.74–2	2
81LUF	300.0–530.0	24	2.00#	0.919	3.89–1	1.84	3.14–2	–2

TABLE 2.87.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C	47	47	0.986	3.01–1	1.43	2.27–2	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
288.1–530.0		3.53509+1	−1.58700+1	4.68941	−4.01211–1		V

TABLE 2.87.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c ($J\,K^{-1}g^{-1}$)	1.61	1.62	1.62	1.63	1.65	1.67	1.68
C ($J\,K^{-1}mol^{-1}$)	158	159	159	160	162	163	165
Temp. (K)	350	360	370	380	390	400	410
c ($J\,K^{-1}g^{-1}$)	1.70	1.72	1.74	1.76	1.78	1.80	1.82
C ($J\,K^{-1}mol^{-1}$)	167	169	171	172	174	176	178
Temp. (K)	420	430	440	450	460	470	480
c ($J\,K^{-1}g^{-1}$)	1.84	1.86	1.88	1.90	1.91	1.93	1.94
C ($J\,K^{-1}mol^{-1}$)	180	182	184	186	187	189	190
Temp. (K)	490	500	510	520	530		
c ($J\,K^{-1}g^{-1}$)	1.95	1.96	1.97	1.97	1.97		
C ($J\,K^{-1}mol^{-1}$)	191	192	193	193	193		



Name: Phosphine
Formula: H_3P

CAS-RN: 7803-51-2
Group No.: 2-088
Molar Mass: 34.00

TABLE 2.88.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36CLU/FRA1	143.2–185.8	9	nosp	not specified		C_p	BSIO	36CLU/GOL
37STE/GIA	146.1–182.7	8	nosp	99.996	melpt	C_p	BSIO	28GIA/WIE1

TABLE 2.88.2. Correlated heat capacities

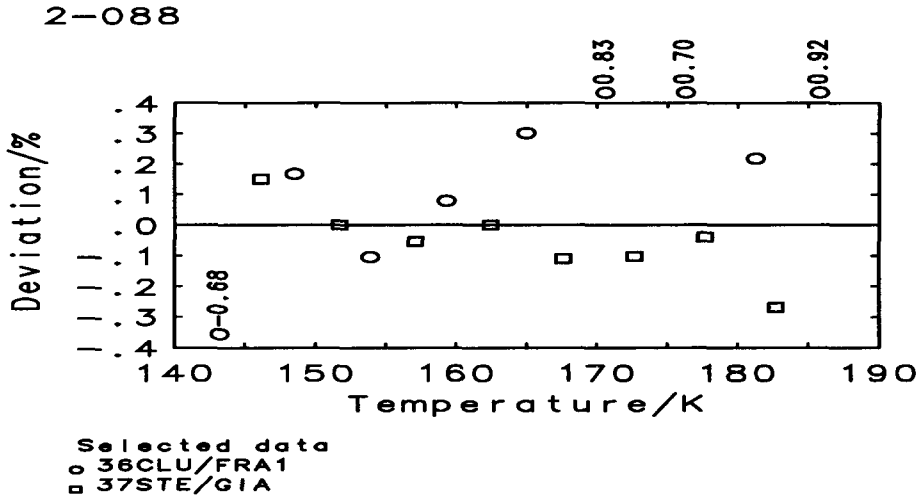
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
36CLU/FRA1	143.2–185.8	9	0.70#	0.775	3.99–2	0.54	1.96–2	5
37STE/GIA	146.1–182.7	8	0.30#	0.414	9.05–3	0.12	–3.95–3	–4

TABLE 2.88.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.696	3.27–2	0.45	8.54–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
143.2–185.8		1.06796+1	–4.08758	1.22669			II

TABLE 2.88.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180
c_p ($J\,K^{-1}g^{-1}$)	1.800	1.787	1.780	1.779	1.784
C_p ($J\,K^{-1}mol^{-1}$)	61.21	60.76	60.53	60.50	60.67



Name: Hydrazine
Formula: H_4N_2

CAS–RN: 302–01–2
Group No.: 2–089
Molar Mass: 32.05

TABLE 2.89.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49SCO/OLI	274.7–340.0	9S	0.30	99.75	melpt	C_{sat}	BSAO	43RUE/HUF
50HOU/MAS1	313.1–353.1	5S	1.00	99.9	anal	C_p	BSAO	50SAG/HOU
68AHL/YOU	331.1–464.1	6	2.00	97.	estim	C_p	FSIO	68AHL/YOU

TABLE 2.89.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
49SCO/OLI	274.7–340.0	9	0.30	0.154	5.60–3	0.05	1.77–3	1
50HOU/MAS1	313.1–353.1	5	1.00	0.604	7.21–2	0.60	–5.55–2	–3
68AHL/YOU	331.1–464.1	6	2.00	0.588	1.52–1	1.18	7.34–2	4

TABLE 2.89.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.492	9.82–2	0.77	8.96–3	2
C_{sat}	20	20	0.500	1.00–1	0.79	9.15–3	1

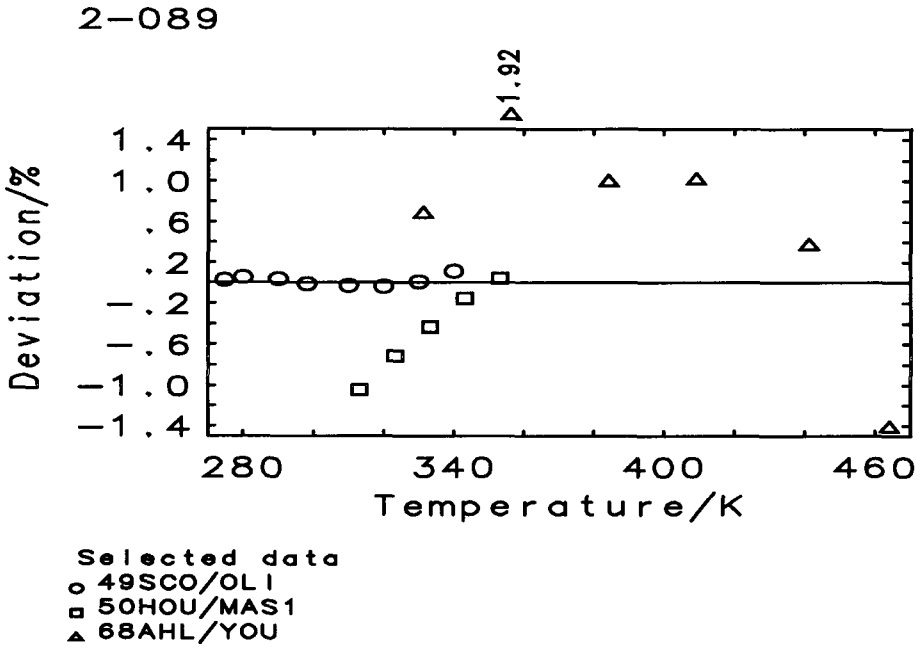
Temp. range K	A_1	A_2	A_3	Level of uncertainty
274.7–464.1	1.10165+1	–1.79459–1	1.58186–1	V
274.7–464.1	1.08647+1	–8.00113–2	1.41975–1	V

TABLE 2.89.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	3.05	3.07	3.08	3.09	3.11	3.13	3.15
C_p (J K^{-1}mol^{-1})	97.7	98.3	98.8	99.0	99.6	100	101
c_{sat} (J K^{-1}g^{-1})	3.05	3.07	3.08	3.09	3.11	3.13	3.15
C_{sat} (J K^{-1}mol^{-1})	97.7	98.3	98.8	99.0	99.6	100	101
Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	3.17	3.20	3.22	3.25	3.27	3.30	3.33
C_p (J K^{-1}mol^{-1})	102	102	103	104	105	106	107
c_{sat} (J K^{-1}g^{-1})	3.17	3.20	3.22	3.25	3.27	3.30	3.33
C_{sat} (J K^{-1}mol^{-1})	102	102	103	104	105	106	107
Temp. (K)	410	420	430	440	450	460	
c_p (J K^{-1}g^{-1})	3.36	3.39	3.42	3.45	3.48	3.51	
C_p (J K^{-1}mol^{-1})	108	109	109	110	112	113	
c_{sat} (J K^{-1}g^{-1})	3.35	3.38	3.41	3.44	3.47	3.50	
C_{sat} (J K^{-1}mol^{-1})	107	108	109	110	111	112	

TABLE 2.89.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.836	1.31–1	1.02	4.63–2	1 1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
274.7–464.1	653.00	–1.03550	6.07044–1	9.92212	4.41589–1		V



Name: Silane
Formula: H_4Si

CAS-RN: 7803–62–5
Group No.: 2–090
Molar Mass: 32.12

TABLE 2.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33CLU	90.3–159.2	15	nosp	not specified		C_{sat}	BSIO	29CLU1

TABLE 2.90.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.852	4.35–2	0.60	4.50–4	3
Temp. range K		A_1	A_2				Level of uncertainty
90.3–159.2		6.96847	3.07401–1				IV

TABLE 2.90.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_{sat} (J K^{-1}g^{-1})	1.876	1.884	1.892	1.899	1.907	1.915	1.923
C_{sat} (J K^{-1}mol^{-1})	60.24	60.50	60.75	61.01	61.26	61.52	61.77
Temp. (K)	160						
c_{sat} (J K^{-1}g^{-1})	1.931						
C_{sat} (J K^{-1}mol^{-1})	62.03						

TABLE 2.90.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.871	4.46–2	0.61	4.35–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
90.3–159.2	508.10	2.61284+1	7.32745	–7.06326–1	2.32922+1		IV

Name: Ammonium hydroxide
Formula: H_5NO

CAS-RN: 1336-21-6
Group No.: 2-091
Molar Mass: 35.05

TABLE 2.91.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53HIL/GIA	N	197.1–290.2	18	nosp	99.62	anal	C_p	BSIO	28GIA/WIE1

53HIL/GIA sample contained 0.33 mol.% Ammonium oxide; results corrected to pure Ammonium hydroxide

TABLE 2.91.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.116	5.77–3	0.03	3.60–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
197.1–290.2		1.69315+1	–1.06230+1	6.56821	–9.45264–1		II

TABLE 2.91.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	3.415	3.520	3.627	3.735	3.844	3.952	4.057
C_p (J K^{-1}mol^{-1})	119.7	123.3	127.1	130.9	134.7	138.5	142.2
Temp. (K)	270	273.15	280	290	298.15		
c_p (J K^{-1}g^{-1})	4.158	4.189	4.254	4.344	4.411		
C_p (J K^{-1}mol^{-1})	145.7	146.8	149.1	152.2	154.6		

Name: Hydrazine mononitrate
Formula: $H_5N_3O_3$

CAS-RN: 13464-97-6
Group No.: 2-092
Molar Mass: 95.06

TABLE 2.92.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86ZHO/CHE	350.0–370.0	3S	0.20	99.86	melpt	C_p	BSAO	83TAN/ZHO

TABLE 2.92.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.021	9.82–4	0.00	–6.36–7	0

Temp. range K	A_1	A_2	Level of uncertainty
350.0–370.0	2.29531+1	1.68377–1	IV

TABLE 2.92.4. Recommended values of heat capacities

Temp. (K)	350	360	370
c_p ($J K^{-1}g^{-1}$)	2.059	2.061	2.062
C_p ($J K^{-1}mol^{-1}$)	195.7	195.9	196.0

Name: Ammonium oxide
Formula: H_8N_2O

CAS-RN: 12161-77-2
Group No.: 2-093
Molar Mass: 52.08

TABLE 2.93.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53HIL/GIA	N	196.8–270.2	14	nosp	99.795	anal	C_p	BSIO	28GIA/WIE1

53HIL/GIA sample contained 0.155 mol.% Ammonium hydroxide; results corrected to pure Ammonium oxide

TABLE 2.93.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	14	14	0.155	1.15–2	0.05	5.72–6	–1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
196.8–270.2	2.15748+1	–7.08088	6.17904	–1.02491	II

TABLE 2.93.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	3.821	3.906	3.990	4.072	4.152	4.227	4.298
C_p (J K^{-1}mol^{-1})	199.0	203.4	207.8	212.1	216.2	220.1	223.8

Temp. (K)	270
c_p (J K^{-1}g^{-1})	4.363
C_p (J K^{-1}mol^{-1})	227.2

Name: Mercury iodide (HgI_2)
Formula: HgI_2

CAS-RN: 7774-29-0
Group No.: 2-094
Molar Mass: 454.40

TABLE 2.94.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
07GUI1	N	523.2-603.0	2	4.00	not specified		C_p	DSIO	07GUI1

07GUI1 values calculated from temperature dependence of enthalpy by the author

TABLE 2.94.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
523.2-603.0	1.26678+1	VI

TABLE 2.94.4. Recommended values of heat capacities

Temp. (K)	530	600
c_p (J K^{-1}g^{-1})	0.23	0.23
C_p (J K^{-1}mol^{-1})	105	105

Name: Tetraiodostannane
Formula: I_4Sn

CAS-RN: 7790-47-8
Group No.: 2-095
Molar Mass: 626.33

TABLE 2.95.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36NEG	N	430.40	0.2679	nosp	not specified		C_{avg}	DSIO	36NEG

36NEG average value in temperature range 418-443 K

Name: Lithium salt nitric acid
Formula: $LiNO_3$

CAS-RN: 7790-69-4
Group No.: 2-096
Molar Mass: 68.95

TABLE 2.96.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
09GOO/KAL	N	523.2–576.2	2	nosp	not specified		C_{avg}	DSIO	09GOO/KAL

09GOO/KAL constant value calculated from temperature dependence of enthalpy by the authors

TABLE 2.96.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
523.2–576.2	1.35309+1	V

TABLE 2.96.4. Recommended values of heat capacities

Temp. (K)	525	575
c ($J K^{-1}g^{-1}$)	1.63	1.63
C ($J K^{-1}mol^{-1}$)	113	113

Name: Nitrogen oxide (NO)
Formula: NO

CAS-RN: 10102-43-9
Group No.: 2-097
Molar Mass: 30.01

TABLE 2.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24EUC/KAR	115.4–117.0	3	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
29JOH/GIA	112.8–120.6	6	1.00	99.999	melpt	C_{sat}	BSIO	28GIA/WIE1
57KER	113.4–155.7	11	nosp	99.999	estim	C_{sat}	BSIO	30WIE/HUB

TABLE 2.97.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
			Selected data					
24EUC/KAR	115.4–117.0	3	3.00	0.262	6.83–2	0.78	5.82–2	3
29JOH/GIA	112.8–120.6	6	1.00	0.941	8.18–2	0.94	–4.30–2	–4
57KER	113.4–155.7	11	0.60#	1.095	9.14–2	0.66	9.44–3	1

TABLE 2.97.3. Parameters of cubic spline polynomials

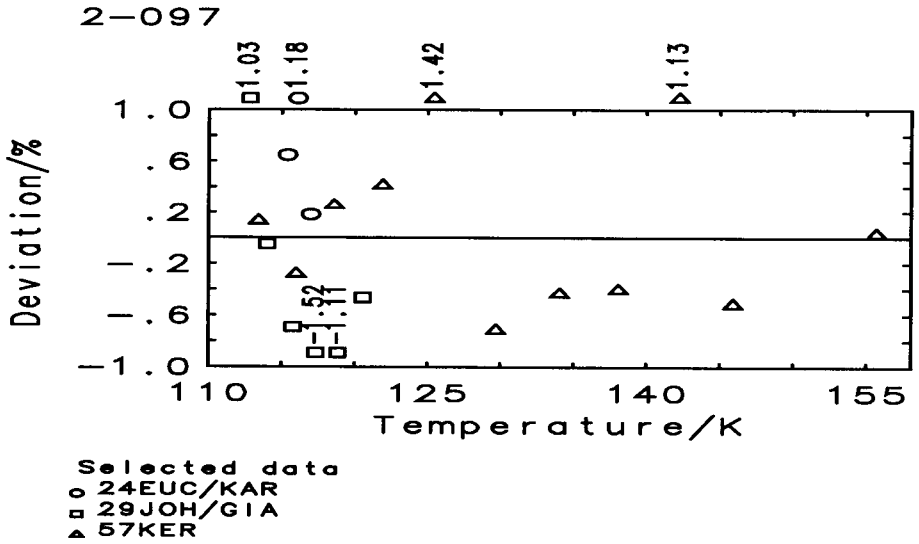
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	20	20	1.117	9.87–2	0.89	1.00–3	0
C_{sat}	20	20	1.119	9.86–2	0.89	1.05–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
112.8–140.0		−4.97348+2	1.25489+3	−1.05137+3	2.97920+2		IV
140.0–155.7		4.50967+3	−9.47444+3	6.61243+3	−1.52680+3		IV
112.8–140.0		−4.90222+2	1.23646+3	−1.03541+3	2.93282+2		IV
140.0–155.7		4.58450+3	−9.63795+3	6.73203+3	−1.55611+3		IV

TABLE 2.97.4. Recommended values of heat capacities

Temp. (K)	110	115	120	125	130	135	140
c_p (J K^{-1}g^{-1})	2.051	2.337	2.590	2.873	3.247	3.774	4.516
C_p (J K^{-1}mol^{-1})	61.53	70.11	77.72	86.21	97.43	113.2	135.5
c_{sat} (J K^{-1}g^{-1})	2.050	2.334	2.586	2.866	3.236	3.755	4.486
C_{sat} (J K^{-1}mol^{-1})	61.51	70.05	77.60	86.01	97.09	112.7	134.6
Temp. (K)	145	150	155				
c_p (J K^{-1}g^{-1})	5.472	6.388	6.945				
C_p (J K^{-1}mol^{-1})	164.2	191.7	208.4				
c_{sat} (J K^{-1}g^{-1})	5.424	6.311	6.824				
C_{sat} (J K^{-1}mol^{-1})	162.8	189.4	204.8				

TABLE 2.97.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	20	20	3.334	2.57–1	2.38	−6.03–2	−6
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
112.8–155.7	180.00	1.84380+2	6.08075	−2.73952+2	1.67806+3	−2.67048+3	1.80793+3	V



Name: Nitrogen oxide (NO_2)
Formula: NO_2

CAS-RN: 10102-44-0
Group No.: 2-098
Molar Mass: 46.01

TABLE 2.98.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50SAG/HOU	294.3–377.6	16	2.00	not specified		C_p	BSAO	50SAG/HOU

TABLE 2.98.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	16	16	0.193	3.61-2	0.39	3.22-4	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
294.3–377.6		6.86227+1	-3.92134+1	6.45157			V

TABLE 2.98.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.66	1.64	1.63	1.64	1.66	1.71	1.79
C_p ($J K^{-1} mol^{-1}$)	76.2	75.3	75.2	75.3	76.5	78.8	82.1
Temp. (K)	350	360	370	380			
c_p ($J K^{-1} g^{-1}$)	1.88	2.00	2.14	2.31			
C_p ($J K^{-1} mol^{-1}$)	86.5	92.0	98.6	106			

Name: Nitrogen oxide (N_2O)
Formula: N_2O

CAS-RN: 10024-97-2
Group No.: 2-099
Molar Mass: 44.01

TABLE 2.99.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
35BLU/GIA	183.6–187.1	5	nosp	99.999	estim	C_{sat}	BSIO	28GIA/WIE1
74ATA/CHI	183.1–184.4	6	nosp	99.999	melpt	C_{sat}	BSAO	74ATA/CHI

TABLE 2.99.2. Correlated heat capacities

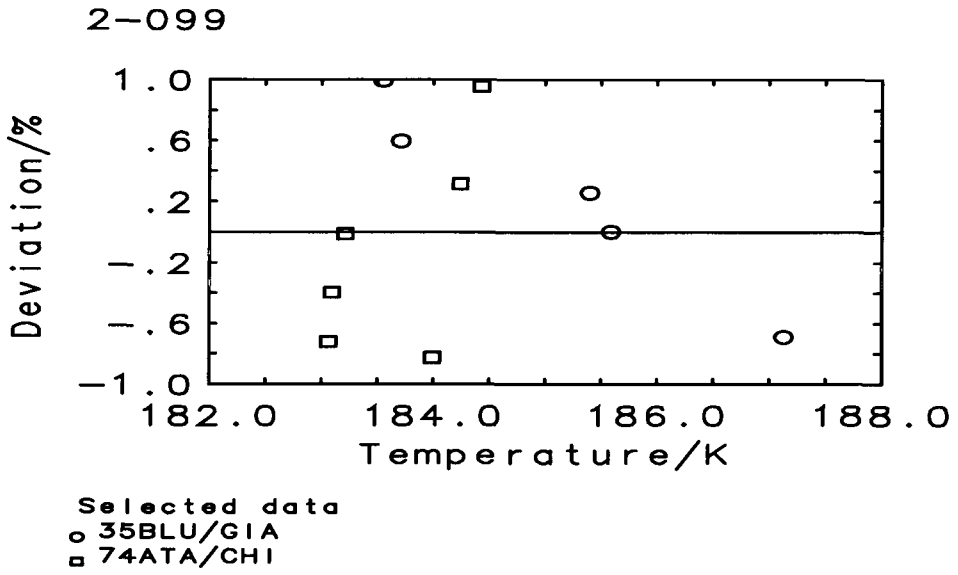
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
			Selected data					
35BLU/GIA	183.6–187.1	5	0.50#	1.227	5.73-2	0.61	2.14-2	2
74ATA/CHI	183.1–184.4	6	0.40#	1.573	5.83-2	0.63	-1.03-2	-2

TABLE 2.99.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	11	11	1.577	6.39–2	0.69	4.10–3	0
Temp. range K		A_1	A_2				Level of uncertainty
183.1–187.1		9.17947–1	4.54050				IV

TABLE 2.99.4. Recommended values of heat capacities

Temp. (K)	183	184	185	186	187
c_{sat} (J K^{-1}g^{-1})	1.743	1.752	1.760	1.769	1.777
C_{sat} (J K^{-1}mol^{-1})	76.72	77.10	77.47	77.85	78.23



Name: Nitrogen oxide (N_2O_4)
Formula: N_2O_4

CAS-RN: 10544–72–6
Group No.: 2–100
Molar Mass: 92.01

TABLE 2.100.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38GIA/KEM	265.4–291.3	6	nosp	99.99	melpt	C_p	BSIO	28GIA/WIE1

TABLE 2.100.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.176	1.47–2	0.09	1.84–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
265.4–291.3	1.14261+1	1.90591	IV

TABLE 2.100.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	1.498	1.503	1.515	1.532	1.546
C_p ($J K^{-1}mol^{-1}$)	137.8	138.3	139.4	141.0	142.2

Name: Sulfur dioxide
Formula: O_2S

CAS-RN: 7446-09-5
Group No.: 2-101
Molar Mass: 64.06

TABLE 2.101.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
37PER2	N	202.3–291.4	23	nosp	not specified	C_{sat}	BSIO	37PER1
38GIA/STE		201.7–260.9	12	0.20	99.999 melpt	C_p	BSIO	37GIA/EGA
39RIE2		233.6–272.9	10	nosp	not specified	C_{sat}	BSIO	39RIE3

37PER2 sample contained traces of water (information in 39RIE2)

TABLE 2.101.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
38GIA/STE	201.7–260.9	12	0.20	0.522	1.09–2	0.10	–3.00–3	–1
39RIE2	233.6–273.0	10	0.70#	0.694	5.11–2	0.49	4.50–2	10
				Rejected data				
37PER2	(2.61–1, 2.43, 2.51–1, 19)							

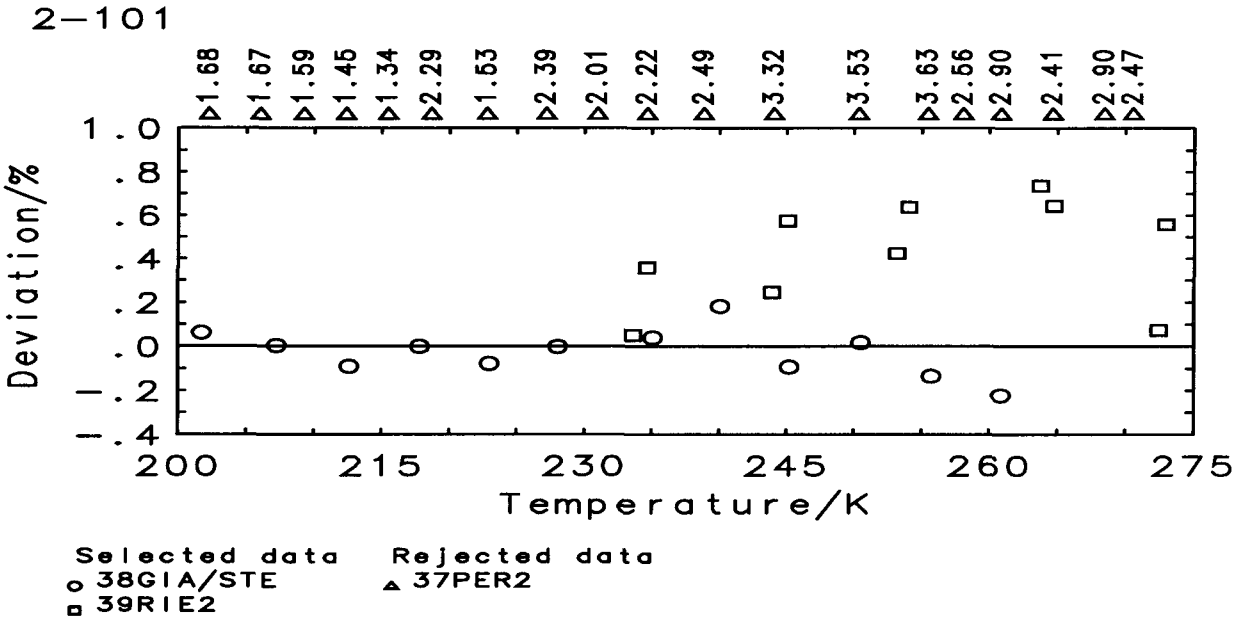
TABLE 2.101.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	22	0.670	3.91–2	0.37	1.88–2	9
C_{sat}	45	22	0.671	3.91–2	0.37	1.89–2	9

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
201.7–273.0	–1.03956+1	2.82843+1	–1.26047+1	1.84895	IV
201.7–273.0	–1.05434+1	2.83858+1	–1.26030+1	1.84108	IV

TABLE 2.101.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J\,K^{-1}g^{-1}$)	1.368	1.364	1.360	1.355	1.353	1.354	1.360
C_p ($J\,K^{-1}mol^{-1}$)	87.62	87.39	87.10	86.83	86.68	86.74	87.11
c_{sat} ($J\,K^{-1}g^{-1}$)	1.368	1.364	1.359	1.355	1.352	1.353	1.358
C_{sat} ($J\,K^{-1}mol^{-1}$)	87.62	87.39	87.09	86.81	86.63	86.66	86.98



Name: Sulfur trioxide
Formula: O_3S

CAS-RN: 7446-11-9
Group No.: 2-102
Molar Mass: 80.06

TABLE 2.102.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type Reference
53GME	N	303.1	1	nosp	not specified	C_{avg}	not specified
76MIL/SCH	N	290.0–473.0	eqn	nosp	not specified	C_p	not specified
89KON/STR	N	290.1–302.0	7S	0.30	not specified	C_{sat}	BSAO 89KON/STR

53GME gamma form; average value in temperature range 298–308 K
76MIL/SCH unspecified origin of experimental data
89KON/STR SO_2 content 0.01 mass %

TABLE 2.102.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76MIL/SCH	311.6–473.6	16	3.00#	1.093	1.34	3.28	–3.07–1	–2
89KON/STR	290.1–302.0	7	0.30	1.305	1.07–1	0.39	8.85–3	–1
				Rejected data				
53GME	(2.12, 6.84, 2.12, 1)							

TABLE 2.102.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	23	1.313	1.26	3.10	–2.11–1	–3
C_{sat}	26	23	1.394	1.35	3.30	–2.11–1	–3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
290.1–305.0	–3.72738+3	3.52845+3	–1.11164+3	1.17580+2	IV
305.0–473.6	–8.91729+2	7.39284+2	–1.97155+2	1.76369+1	V
290.1–305.0	–4.31398+3	4.11091+3	–1.30428+3	1.38804+2	IV
305.0–473.6	–8.34788+2	6.88754+2	–1.82265+2	1.61787+1	V

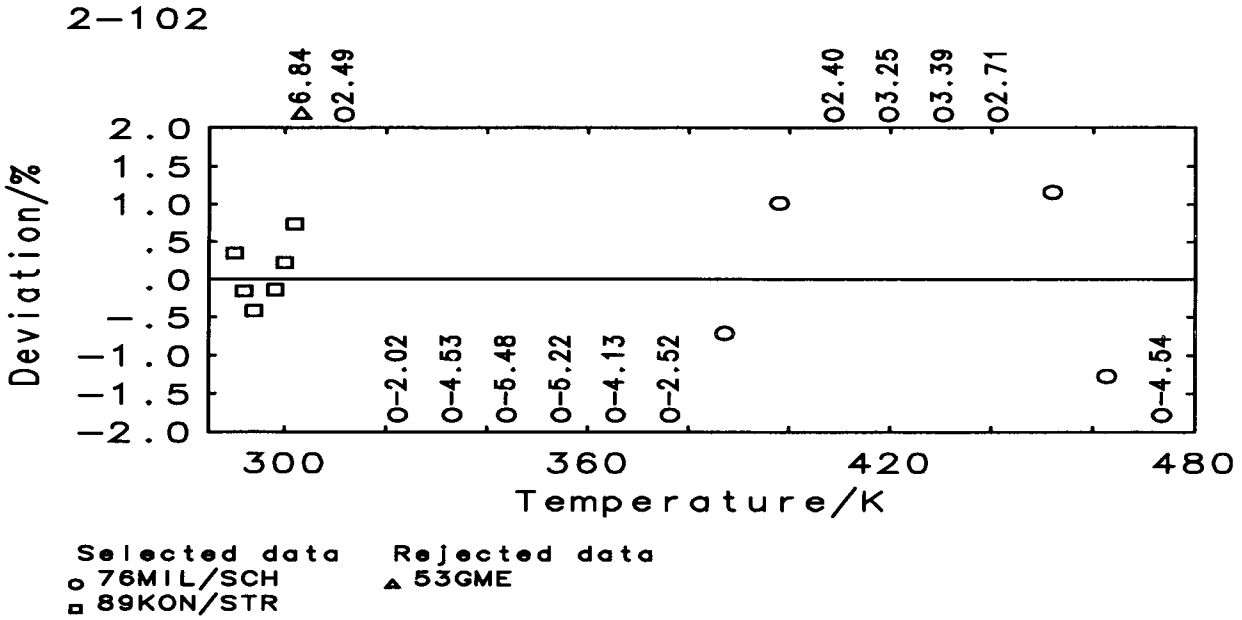
TABLE 2.102.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	2.485	2.833	2.898	3.20	3.43	3.60	3.73
C_p ($J K^{-1} mol^{-1}$)	199.0	226.8	232.1	256	275	289	299
c_{sat} ($J K^{-1} g^{-1}$)	2.484	2.832	2.897	3.19	3.42	3.60	3.73
C_{sat} ($J K^{-1} mol^{-1}$)	198.9	226.7	232.0	256	274	288	298
Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1} g^{-1}$)	3.82	3.89	3.94	3.99	4.05	4.12	4.23
C_p ($J K^{-1} mol^{-1}$)	306	311	315	319	324	330	338
c_{sat} ($J K^{-1} g^{-1}$)	3.82	3.88	3.94	3.98	4.03	4.09	4.18
C_{sat} ($J K^{-1} mol^{-1}$)	306	311	315	319	323	328	335
Temp. (K)	420	430	440	450	460	470	
c_p ($J K^{-1} g^{-1}$)	4.38	4.57	4.84	5.17	5.60	6.11	
C_p ($J K^{-1} mol^{-1}$)	350	366	387	414	448	489	
c_{sat} ($J K^{-1} g^{-1}$)	4.31	4.48	4.70	4.99	5.35	5.80	
C_{sat} ($J K^{-1} mol^{-1}$)	345	358	376	399	428	464	

TABLE 2.102.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	23	12.610	1.80	5.94	5.09–1	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
290.1–473.6	491.00	–3.41225	2.63366–2	2.06294+1	–2.28477	–1.45276+1	4.60172+1	VI



Name: Phosphorus oxide P_4O_6
Formula: O_6P_4

CAS–RN: 12440–00–5
Group No.: 2–103
Molar Mass: 219.89

TABLE 2.103.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86KAU/HEI	298.00	0.9509	0.65	not specified		C_p	BSIO	86KAU/HEI

1. Compounds of Carbon and Hydrogen

11. Saturated Aliphatic Hydrocarbons

This family consists of 83 saturated aliphatic hydrocarbons; for 7 compounds data are available at a single temperature only. A survey of experimental sources and the recommended data for the C_1 to C_{18} n-alkanes have been recently published (91RUZ/ZAB). For these compounds, some newer measurements have been considered when establishing recommendations for this monograph.

Most of the measurements in this family were performed at BMB in connection with investigations of properties of compounds contained in petroleum and coal. A total of 33 hydrocarbons containing five or more carbon atoms were measured in an adiabatic calorimeter (43RUE/HUF, stated measurement error of 0.2 %) using high purity samples (43GUT/HUF, 46DOU/HUF2, 52SCO/DOU, 54FIN/GRO2, 61HUF/GRO, 61MCC/MES, 67MES/GUT, 71MES/FIN, 73FIN/MES, 76FIN/MES). In view of the high reliability of these sources, all the data have been selected for the generation of recommended values.

NBSW is another laboratory that was systematically involved in the measurement of the heat capacities of alkanes. Osborne and Ginnings (47OSB/GIN) published data for 11 compounds determined over a narrow temperature interval (20 K) with a claimed error of 0.1 %. All the experimental values have been considered in the final selection for producing the recommended data. More recent measurements were carried out over a wide temperature range at NBSB using a spherical adiabatic calorimeter (61GOO). The measurements were carried out for C_1 to C_3 n-alkane (74YOU, 76ROD2, 78GOO) hydrocarbons from the melting temperature to the critical temperature with the stated measurement error around 0.5 %. These results have been the basis for recommendations and have been supplemented by accurate data from NRCO (65CUT/MOR) and from UCB (37WIT/KEM, 38KEM/EGA).

The low-temperature data for some C_4 hydrocarbons and 2,2-dimethylpropane obtained at the PSC (36AST/MES, 40AST/KEN, 40AST/MES) have been the basis for recommendations and have been supplemented by the superambient data from CITP (35SAG/LAC, 38SAG/LAC). The latter data are of lower accuracy as they were obtained by conversion from the high-pressure measurements. The data from the CITP have been also used for extending the temperature interval of the correlation for some other compounds (50AUE/SAG, 51CON/SAG).

The data from GPI for higher n-alkanes at superambient temperatures (75GRI/RAS, 82KUZ/KHA, 84GRI/AND, 88KUZ/KHA) have been mainly used for extending the low-temperature data from other sources to higher temperatures. The measurement error of 0.9 % reported by the authors is reasonable, and the data are fully compatible with other selected sources. This is not, however, the case for the data from APIB (76MUS, 77NAZ/MUS), where the reported error was much lower than the differences from other reliable data sources. The APIB data have been generally discarded with the exception of high-temperature values for dodecane where no other data were available.

Results for n-hexane from PASW (80KAL/JED) with a reported error of 0.2 % have been selected for the final correlation. Similarly, the data published for C_9, C_{11} and C_{16} n-alkanes from IITD (91BAN/GAR) having a reported error of 0.4 % have been considered as reliable and included in the final selection.

In the 1930's and the beginning of the 1940's, a laboratory at SUC (31HUF/PAR) was involved in the systematic measurement of heat capacities for a variety of organic compounds. Results gave reported errors of around 1 %. The data from this source have been considered when no other values were available for the following: 2,7-dimethyloctane (30PAR/HUF), C_{25} and C_{33} n-alkanes (32SPA/THO), and four isomers of methylnonanes (41PAR/WES). In the case of n-hexane, the values from SUC have been also included in the final correlation as they exhibited good agreement with other selected sources.

Measurements of heat capacities of n-heptane are very frequent as n-heptane is the calorimetric standard (solid and liquid) in the temperature range from 0 to 400 K. Very often this substance was used for calibration purposes or for testing the performance of a calorimeter. Data of this type are numerous in literature and have not been compiled by us. The recommended data for n-heptane as a calorimetric standard were originally established in the temperature range from 182.6 K to 400 K by Ginnings and Furukawa at NBSW (53GIN/FUR). In the liquid phase, the data were based on their extensive measurements performed in an adiabatic calorimeter from 185 K up to 370 K and on data from a drop calorimeter at higher temperatures up to 520 K (54DOU/FUR). These data have been supplemented in the temperature range between 280 and 360 K by additional data from another adiabatic calorimeter (47OSB/GIN). New recommendations for liquid n-heptane in the temperature range from the triple point temperature 182.603 K up to 480 K have been recently published by Zábranský and Růžička (94ZAB/RUZ). The new recommendations also considered the accurate data from BMB (61MCC/MES) summarized in the reference (61HUF/GRO) in addition to data from the above two sources. In all three sources of experimental data, detailed information is available regarding the performance of experiments and raw results; this made it possible to convert the original data to the actually valid temperature scale ITS-90. For more general discussion of conversion between different temperature scales see chapter 5.6. The parameters of cubic splines describing the recommended data for n-heptane in this monograph are identical with those published in the reference (94ZAB/RUZ). In addition, the parameters of a quasi-polynomial equation are also given for a larger temperature range up to the vicinity of the critical temperature.

No experimental data are available for branched alkanes higher than C_{11} with the exception of 11-decyleicosane. This compound was measured independently at SUC and at PSC (45FIS/MAY) with data from the two laboratories in good agreement.

There is also a lack of reliable data for n-alkanes higher than C_{19} with the single exception of n-hexacosane $C_{26}H_{54}$. This compound was measured over a narrow temperature interval of 26 K at NPLT (76AND/MAR). All remaining studies

present usually experimental data on several higher molar mass n-alkanes and the reliability of results is low (48MAZ, 69ATK/LAR, 81HOE). This also holds true for data from Laboratoire de Thermodynamique, INPL-ENSIC, Nancy, France (93DUR/AOU), where a DSC calorimeter (SETARAM) was used for measurements of n-alkanes from C_{18} to C_{50}, with two branched alkanes C_{19} and squalane C_{30}; here, the uncertainty in the data is up to 5 %.

Name: Methane-d_4
Formula: CD_4

CAS-RN: 558-20-3
Group No.: 11-001
Molar Mass: 20.07

TABLE 11.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
40CLU/POP	92.0–108.9	9	nosp	99.2	melpt	C_p	BSIO	40CLU/POP
63COL/GIL	91.0–95.0	3	nosp	99.995	chrom	C_p	BSAO	61FLU/LEA

TABLE 11.1.2. Correlated heat capacities

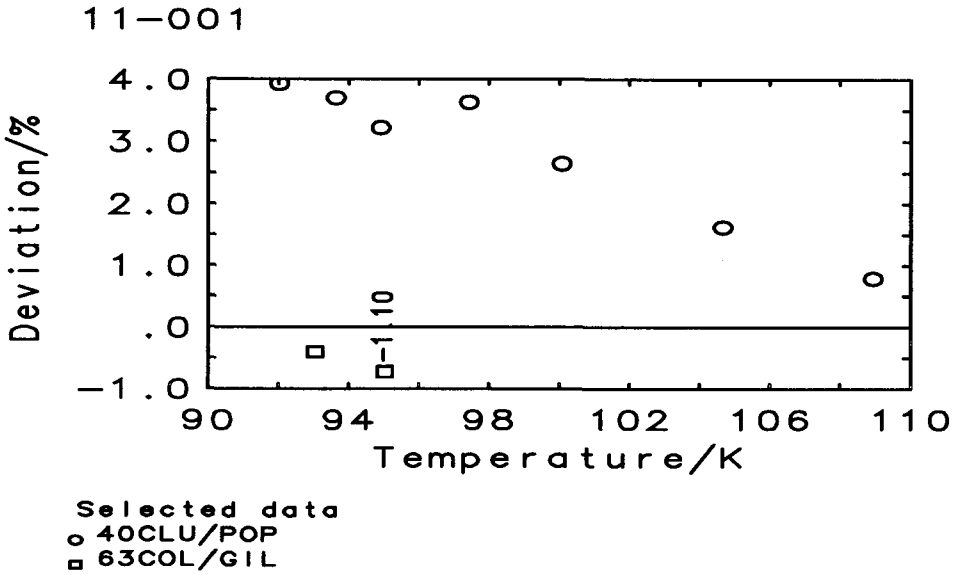
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40CLU/POP	92.0–108.9	9	3.00#	1.033	2.12–1	3.10	2.00–1	9
63COL/GIL	91.0–95.0	3	0.60#	1.227	4.80–2	0.74	–2.18–2	–1

TABLE 11.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	1.189	2.02–1	2.97	1.45–1	8
Temp. range K		A_1	A_2				Level of uncertainty
91.0–108.9		4.51684	2.17371				V

TABLE 11.1.4. Recommended values of heat capacities

Temp. (K)	90	95	100	105	110
c_p ($J K^{-1} g^{-1}$)	2.68	2.73	2.77	2.82	2.86
C_p ($J K^{-1} mol^{-1}$)	53.8	54.7	55.6	56.5	57.4



Name: Methane-*d*
Formula: CH_3D

CAS-RN: 676-49-3
Group No.: 11-002
Molar Mass: 17.05

TABLE 11.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
40CLU/POP	92.5–100.3	13	nosp	99.3	anal	C_p	BSIO	40CLU/POP

TABLE 11.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	13	13	1.034	6.86-2	1.03	1.20-3	-1
Temp. range K		A_1	A_2				Level of uncertainty
92.5–100.3		4.88467	1.79811				V

TABLE 11.2.4. Recommended values of heat capacities

Temp. (K)	92.50	95	97.50	100
c_p (J $K^{-1}g^{-1}$)	3.19	3.22	3.24	3.26
C_p (J $K^{-1}mol^{-1}$)	54.4	54.8	55.2	55.6

Name: Methane
Formula: CH_4

CAS–RN: 74–82–8
Group No.: 11–003
Molar Mass: 16.04

TABLE 11.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24EUC/KAR	96.3–108.7	7	3.00	not specified		C_{sat}	BSIO	24EUC/KAR
29CLU1	95.4–105.3	6	0.70	not specified		C_p	BSIO	29CLU1
30WIE/BRE	110.9–188.2	18	2.00	not specified		C_{sat}	BSIO	30WIE/HUB
61HES/WHI	114.5–187.5	9	nosp	99.96	melpt	C_{sat}	BSIO	53RIF/KER
63COL/GIL	93.4	1	nosp	99.995	chrom	C_p	BSAO	61FLU/LEA
65CUT/MOR	93.9–107.0	5	0.20	99.98	chrom	C_{sat}	BSAO	61FLU/LEA
74YOU	95.4–187.6	66	0.50	99.99	melpt	C_{sat}	BSAO	61GOO

TABLE 11.3.2. *Correlated heat capacities*

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
29CLU1	95.4–105.3	5	0.70	0.390	1.78–2	0.27	–5.19–3	–1
63COL/GIL	93.4	1	0.70#	0.597	2.66–2	0.42	–2.66–2	–1
65CUT/MOR	93.9–107.0	4	0.20	2.718	3.54–2	0.54	–2.93–2	–4
74YOU	95.4–184.2	61	0.50	2.294	1.24–1	1.15	1.62–2	12
				Rejected data				
24EUC/KAR	(2.79–1, 4.09, 2.67–1, 7)			30WIE/BRE	(1.11–1, 1.21, –9.50–2, –14)			
61HES/WHI	(4.32–1, 3.38, 2.76–1, 6)							

TABLE 11.3.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	112	71	2.344	1.21–1	1.13	1.15–2	6
C_{sat}	112	71	1.888	8.00–2	0.90	9.98–3	7

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
93.4–120.0	–7.80294	3.79280+1	–3.44502+1	1.08305+1	III
120.0–150.0	1.43599+1	–1.74792+1	1.17225+1	–1.99521	III
150.0–180.0	–4.62540+2	9.36320+2	–6.24144+2	1.39308+2	IV
180.0–184.2	–1.68405+5	2.80841+5	–1.56127+5	2.89361+4	V
93.4–120.0	2.20300–1	1.55051+1	–1.36198+1	4.39165	III
120.0–150.0	6.34746	1.87213–1	–8.54884–1	8.45838–1	III
150.0–180.0	–2.79355+2	5.71593+2	–3.81792+2	8.54985+1	IV
180.0–184.2	–9.66777+4	1.61236+5	–8.96395+4	1.66147+4	V

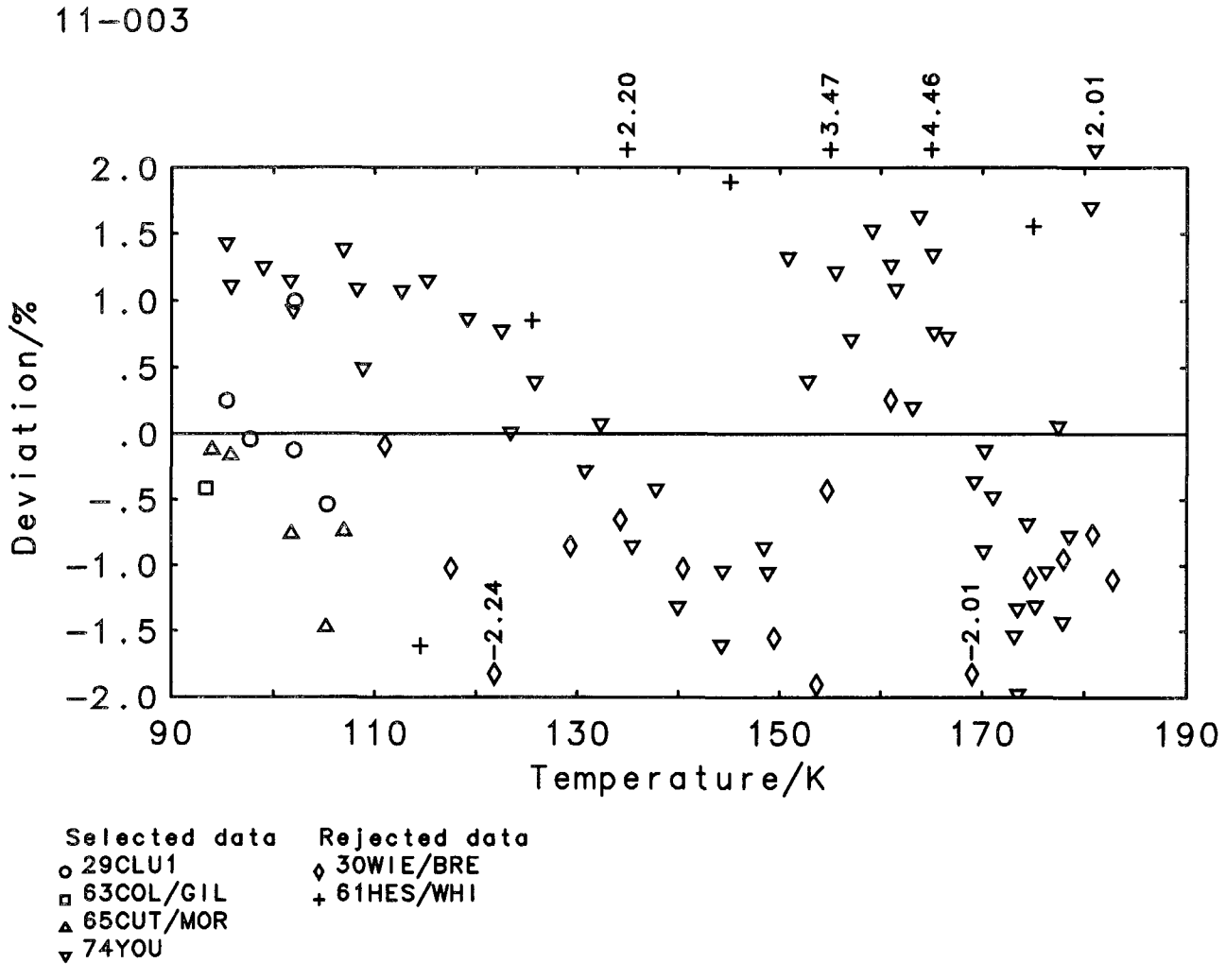
TABLE 11.3.4. Recommended values of heat capacities

Temp. (K)	100	110	120	130	140	150	160
c_p ($J K^{-1}g^{-1}$)	3.372	3.446	3.533	3.661	3.830	4.034	4.339
C_p ($J K^{-1}mol^{-1}$)	54.09	55.28	56.68	58.74	61.45	64.71	69.61
c_{sat} ($J K^{-1}g^{-1}$)	3.367	3.442	3.526	3.630	3.760	3.918	4.150
C_{sat} ($J K^{-1}mol^{-1}$)	54.02	55.22	56.56	58.24	60.32	62.85	66.58

Temp. (K)	170	180
c_p ($J K^{-1}g^{-1}$)	5.106	6.767
C_p ($J K^{-1}mol^{-1}$)	81.91	108.6
c_{sat} ($J K^{-1}g^{-1}$)	4.679	5.770
C_{sat} ($J K^{-1}mol^{-1}$)	75.06	92.57

TABLE 11.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	112	71	1.895	5.98–2	0.71	–1.95–3	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
93.4–184.2	190.55	–1.14331	3.00241–1	5.99170	–1.42092	–1.21632	1.01112	IV



Name: Ethane
Formula: C_2H_6

CAS–RN: 74–84–0
Group No.: 11–004
Molar Mass: 30.07

TABLE 11.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
28EUC/HAU		100.0–270.0	18S	nosp	not specified		C_{sat}	BSIO	28EUC/HAU
30WIE/HUB	N	96.8–138.2	15	1.00	99.0	estim	C_{sat}	BSIO	30WIE/HUB
37WIT/KEM		91.6–180.9	29	0.40	99.5	melpt	C_p	BSIO	28GIA/WIE1
76ROD1		92.2	1	nosp	not specified		C_p	BSAO	61GOO
76ROD2		93.7–301.5	106	0.50	99.98	chrom	C_{sat}	BSAO	61GOO

30WIE/HUB error below and above n.b.t. 0.5 % and 1.0 %, respectively

TABLE 11.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
30WIE/HUB	96.8–138.2	15	1.00	0.423	3.52–2	0.42	4.33–3	2
37WIT/KEM	91.6–180.9	29	0.40	0.943	3.21–2	0.38	4.88–3	12
76ROD1	92.2	1	0.30#	1.511	3.73–2	0.45	3.73–2	1
76ROD2	93.7–300.5	105	0.50	1.524	1.21–1	0.76	–8.65–4	–14
				Rejected data				
28EUC/HAU	(1.70, 15.55, 1.64, 18)							

TABLE 11.4.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	169	150	1.386	1.05–1	0.69	1.02–3	1
C_{sat}	169	150	1.017	6.46–2	0.50	1.59–4	–5

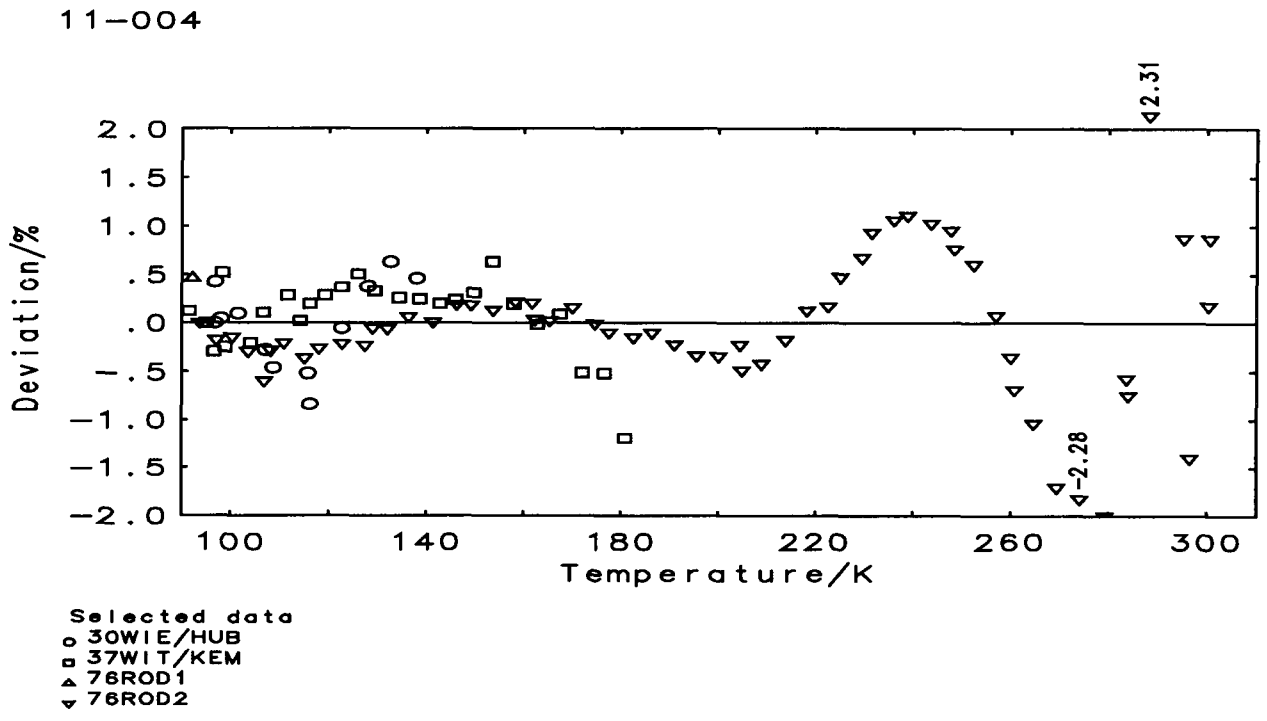
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
91.6–150.0	5.15482	7.37389	–5.93045	1.64512	III
150.0–220.0	1.16122+1	–5.54078	2.67933	–2.68162–1	III
220.0–285.0	–1.45955+2	2.09323+2	–9.49860+1	1.45296+1	IV
285.0–300.6	–6.63205+4	6.98668+4	–2.45362+4	2.87315+3	V
91.6–150.0	5.78529	5.82763	–4.69303	1.32210	III
150.0–220.0	1.08828+1	–4.36730	2.10359	–1.88259–1	III
220.0–285.0	–9.30994+1	1.37427+2	–6.23482+1	9.57716	IV
285.0–300.6	–3.81156+4	4.01611+4	–1.41057+4	1.65208+3	V

TABLE 11.4.4. Recommended values of heat capacities

Temp. (K)	100	110	120	130	140	150	160
c_p ($J K^{-1}g^{-1}$)	2.279	2.289	2.297	2.304	2.314	2.329	2.352
C_p ($J K^{-1}mol^{-1}$)	68.54	68.84	69.06	69.28	69.58	70.05	70.74
c_{sat} ($J K^{-1}g^{-1}$)	2.279	2.289	2.296	2.305	2.315	2.331	2.353
C_{sat} ($J K^{-1}mol^{-1}$)	68.53	68.82	69.05	69.30	69.62	70.09	70.75
Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1}g^{-1}$)	2.383	2.421	2.466	2.517	2.574	2.637	2.708
C_p ($J K^{-1}mol^{-1}$)	71.66	72.80	74.15	75.68	77.40	79.28	81.43
c_{sat} ($J K^{-1}g^{-1}$)	2.382	2.417	2.457	2.504	2.556	2.613	2.678
C_{sat} ($J K^{-1}mol^{-1}$)	71.61	72.66	73.90	75.30	76.87	78.58	80.53
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	2.809	2.963	3.194	3.527	3.657	3.985	4.69
C_p ($J K^{-1}mol^{-1}$)	84.46	89.09	96.05	106.1	110.0	119.8	141
c_{sat} ($J K^{-1}g^{-1}$)	2.763	2.885	3.059	3.302	3.395	3.629	4.11
C_{sat} ($J K^{-1}mol^{-1}$)	83.09	86.75	91.99	99.29	102.1	109.1	124
Temp. (K)	298.15	300					
c_p ($J K^{-1}g^{-1}$)	7.01	8.04					
C_p ($J K^{-1}mol^{-1}$)	211	242					
c_{sat} ($J K^{-1}g^{-1}$)	5.52	6.13					
C_{sat} ($J K^{-1}mol^{-1}$)	166	184					

TABLE 11.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	169	150	0.817	8.00–2	0.40	–1.34–3	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
91.6–300.5	305.33	–2.17287	2.58198–1	7.94568	–1.95607	–3.99364	3.70838	IV



Name: Propane
Formula: C_3H_8

CAS–RN: 74–98–6
Group No.: 11–005
Molar Mass: 44.10

TABLE 11.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26DAN/JEN	241.8–291.6	12	2.00	not specified		C_{sat}	BSIO	26DAN/JEN
38KEM/EGA	89.7–229.8	22	nosp	99.9	melpt	C_p	BSIO	28GIA/WIE1
65CUT/MOR	91.1–104.8	7	0.20	99.99	chrom	C_{sat}	BSAO	61FLU/LEA
78GOO	81.1–288.8	78	2.00	99.99	melpt	C_{sat}	BSAO	61GOO

TABLE 11.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
38KEM/EGA	89.7–229.8	22	0.50#	0.512	2.76–2	0.26	8.07–4	1
65CUT/MOR	91.1–104.8	7	0.20	1.678	3.40–2	0.34	–1.75–2	–3
78GOO	81.1–288.8	78	0.50#	0.501	2.57–2	0.25	9.87–3	34
				Rejected data				
26DAN/JEN	(4.88–1, 4.02, –3.47–1, –9)							

TABLE 11.5.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	119	107	0.668	2.75–2	0.27	6.22–3	32
C_{sat}	119	107	0.668	2.75–2	0.27	6.22–3	34

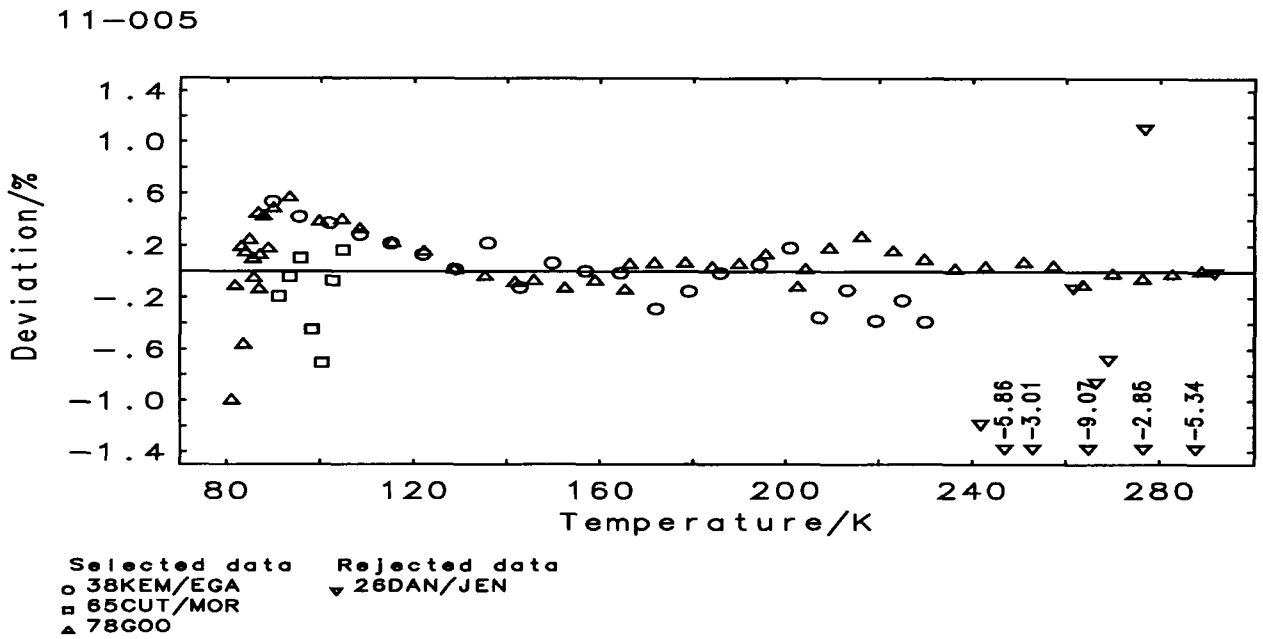
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
81.1–115.0	1.06718+1	–2.47874	2.76584	–7.79883–1	III
115.0–200.0	8.91893	2.09400	–1.21047	3.72671–1	III
200.0–288.8	8.45191	2.79454	–1.56074	4.31049–1	III
81.1–115.0	1.06179+1	–2.32023	2.61241	–7.31099–1	III
115.0–200.0	8.96953	1.97996	–1.12687	3.52752–1	III
200.0–288.8	9.77871	7.66188–1	–5.19990–1	2.51605–1	III

TABLE 11.5.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_p ($J K^{-1}g^{-1}$)	1.907	1.919	1.933	1.948	1.964	1.980	1.998
C_p ($J K^{-1}mol^{-1}$)	84.08	84.63	85.26	85.91	86.59	87.31	88.09
c_{sat} ($J K^{-1}g^{-1}$)	1.907	1.919	1.933	1.948	1.964	1.980	1.998
C_{sat} ($J K^{-1}mol^{-1}$)	84.08	84.63	85.25	85.91	86.59	87.31	88.09
Temp. (K)	160	170	180	190	200	210	220
c_p ($J K^{-1}g^{-1}$)	2.017	2.039	2.063	2.090	2.121	2.155	2.194
C_p ($J K^{-1}mol^{-1}$)	88.94	89.89	90.96	92.16	93.51	95.03	96.75
c_{sat} ($J K^{-1}g^{-1}$)	2.017	2.039	2.063	2.090	2.120	2.154	2.192
C_{sat} ($J K^{-1}mol^{-1}$)	88.94	89.90	90.96	92.15	93.49	94.99	96.67
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	2.238	2.287	2.342	2.403	2.471	2.494	2.546
C_p ($J K^{-1}mol^{-1}$)	98.67	100.8	103.3	106.0	109.0	110.0	112.3
c_{sat} ($J K^{-1}g^{-1}$)	2.235	2.282	2.333	2.390	2.453	2.474	2.521
C_{sat} ($J K^{-1}mol^{-1}$)	98.54	100.6	102.9	105.4	108.2	109.1	111.2
Temp. (K)	290	298.15	300				
c_p ($J K^{-1}g^{-1}$)	2.629	2.703	2.720				
C_p ($J K^{-1}mol^{-1}$)	115.9	119.2	120.0				
c_{sat} ($J K^{-1}g^{-1}$)	2.595	2.660	2.676				
C_{sat} ($J K^{-1}mol^{-1}$)	114.4	117.3	118.0				

TABLE 11.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	119	107	0.856	3.75–2	0.33	–3.53–3	–16
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
81.1–288.8	369.85	–4.67531–1	1.02374	8.63274	5.33790–2		III



Name: Butane
Formula: C_4H_{10}

CAS–RN: 106–97–8
Group No.: 11–006
Molar Mass: 58.12

TABLE 11.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26DAN/JEN		256.9–294.4	10	2.00	not specified		C_{sat}	BSIO	26DAN/JEN
31HUF/PAR		139.7–261.8	8	1.00	not specified		C_p	BSIO	25PAR
35SAG/LAC	N	295.4–365.0	18	nosp	99.21	anal	C_{sat}	BSAO	35SAG/LAC
40AST/MES		139.9–268.1	21	nosp	99.999	melpt	C_p	BSIO	36AST/MES

35SAG/LAC data from a graph only

TABLE 11.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
35SAG/LAC	295.4–365.0	18	1.50#	0.811	2.21–1	1.22	–3.53–2	–4
40AST/MES	139.9–268.1	21	0.30#	1.070	4.78–2	0.32	1.70–3	–3
				Rejected data				
26DAN/JEN	(3.72–1, 2.22, 1.58–1, 4)			31HUF/PAR	(1.04–1, 0.73, –9.38–2, –7)			

TABLE 11.6.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	57	39	1.043	1.67–1	0.93	–1.54–2	–7
C_{sat}	57	39	1.041	1.67–1	0.94	–1.56–2	–7

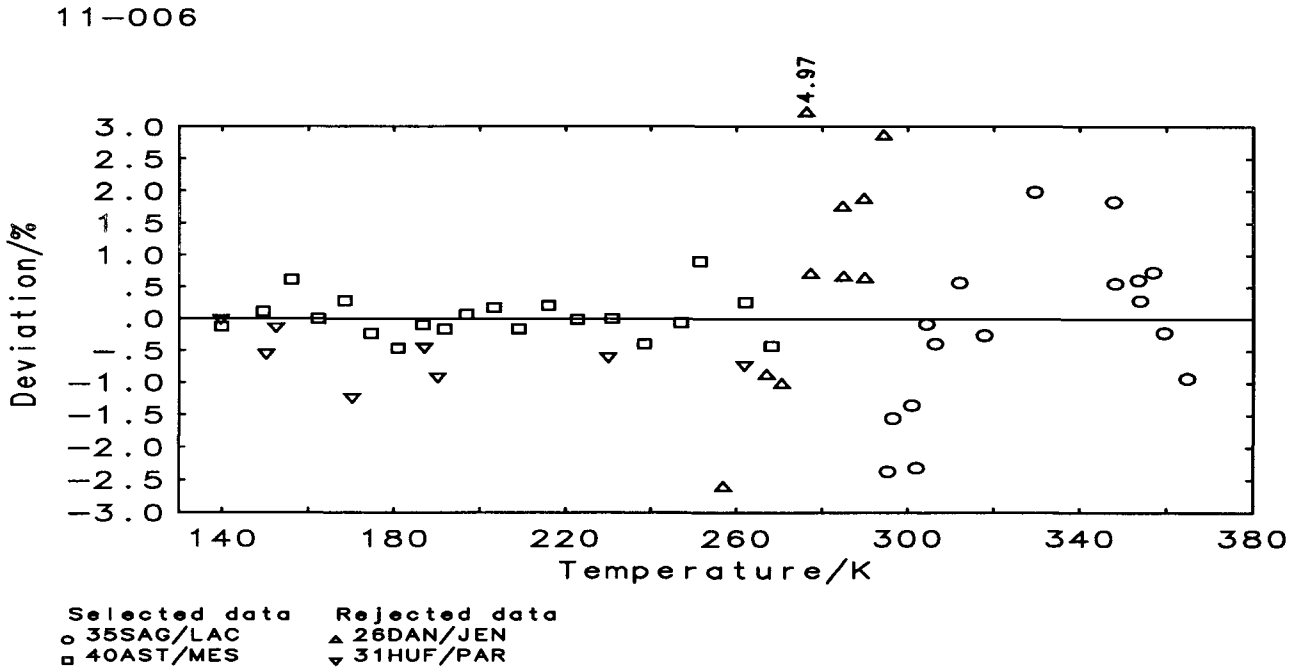
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
139.9–210.0	4.83762	1.35958+1	–7.10150	1.34439	III
210.0–300.0	1.67875+1	–3.47554	1.02771	5.40420–2	IV
300.0–365.0	–9.55521+1	1.08864+2	–3.64188+1	4.21477	V
139.9–210.0	4.97370	1.33646+1	–6.97262	1.32080	III
210.0–300.0	1.72549+1	–4.17994	1.38194	–5.31594–3	IV
300.0–365.0	–7.32884+1	8.63633+1	–2.87991+1	3.34814	V

TABLE 11.6.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p (J K^{-1}g^{-1})	1.951	1.973	1.991	2.007	2.023	2.039	2.057
C_p (J K^{-1}mol^{-1})	113.4	114.7	115.7	116.7	117.6	118.5	119.5
c_{sat} (J K^{-1}g^{-1})	1.951	1.973	1.991	2.007	2.023	2.039	2.057
C_{sat} (J K^{-1}mol^{-1})	113.4	114.7	115.7	116.7	117.6	118.5	119.6
Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	2.077	2.102	2.130	2.162	2.198	2.238	2.283
C_p (J K^{-1}mol^{-1})	120.7	122.1	123.8	125.7	127.8	130.1	132.7
c_{sat} (J K^{-1}g^{-1})	2.077	2.102	2.130	2.161	2.197	2.237	2.280
C_{sat} (J K^{-1}mol^{-1})	120.7	122.1	123.8	125.6	127.7	130.0	132.5
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.298	2.332	2.385	2.431	2.442	2.50	2.57
C_p (J K^{-1}mol^{-1})	133.6	135.5	138.6	141.3	141.9	146	150
c_{sat} (J K^{-1}g^{-1})	2.294	2.327	2.378	2.423	2.433	2.49	2.56
C_{sat} (J K^{-1}mol^{-1})	133.4	135.3	138.2	140.8	141.4	145	149
Temp. (K)	330	340	350	360			
c_p (J K^{-1}g^{-1})	2.66	2.75	2.87	3.01			
C_p (J K^{-1}mol^{-1})	154	160	167	175			
c_{sat} (J K^{-1}g^{-1})	2.63	2.72	2.82	2.95			
C_{sat} (J K^{-1}mol^{-1})	153	158	164	171			

TABLE 11.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	57	39	4.651	2.49–1	1.62	9.50–2	15
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
139.9–365.0	425.25	–2.13769	7.79723–1	1.07168+1	1.46518		V



Name: 2–Methylpropane
Formula: C_4H_{10}

CAS–RN: 75–28–5
Group No.: 11–007
Molar Mass: 58.12

TABLE 11.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26DAN/JEN	259.4–290.6	11	2.00	not specified		C_{sat}	BSIO	26DAN/JEN
37PAR/SHO	115.4–258.3	19	0.70	99.7	melpt	C_p	BSIO	25PAR
38SAG/LAC	294.3–377.6	6S	1.00	99.97	anal	C_p	BSAO	35SAG/LAC
40AST/KEN	116.9–257.0	25	nosp	99.9985	melpt	C_p	BSIO	36AST/MES

TABLE 11.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37PAR/SHO	115.4–258.3	19	0.70	0.472	4.67–2	0.33	–2.58–2	–5
38SAG/LAC	294.3–377.6	6	1.00	0.712	1.24–1	0.71	–6.06–2	–4
40AST/KEN	116.9–257.0	25	0.40#	0.844	4.81–2	0.34	9.24–3	5
				Rejected data				
26DAN/JEN	(1.18, 6.65, 5.76–1, 5)							

TABLE 11.7.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	61	50	0.747	6.52–2	0.42	–1.25–2	–4
C_{sat}	61	50	0.724	6.54–2	0.43	–1.21–2	–2

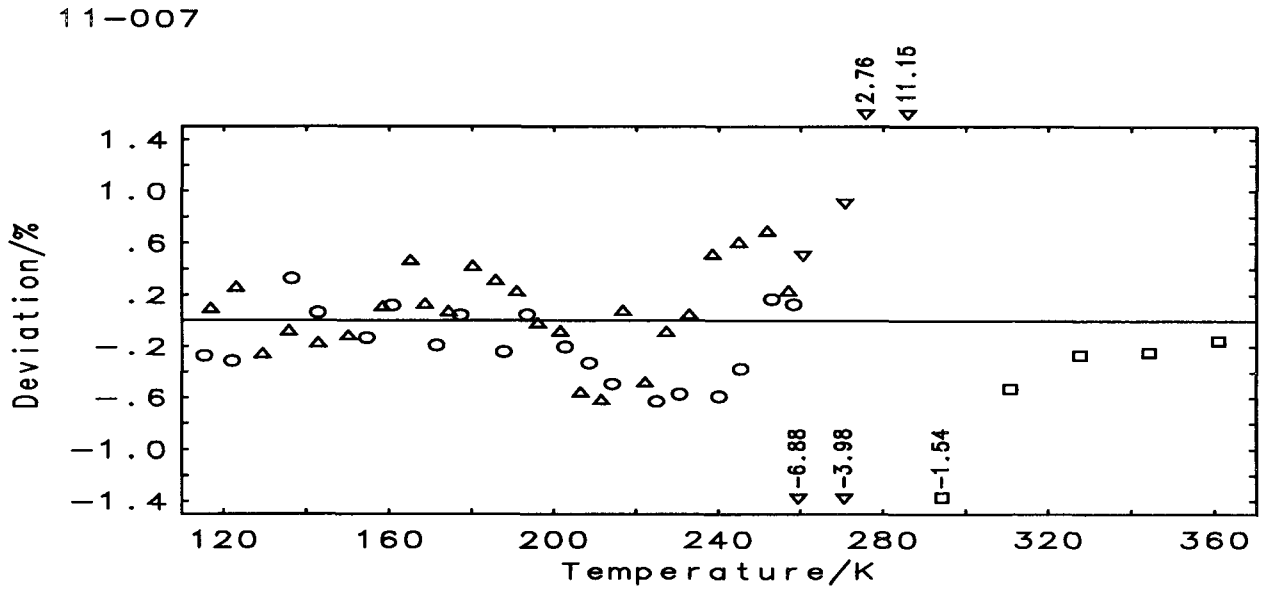
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
115.4–250.0	1.11419+1	–3.29263–1	1.03263	–1.01518–1	III
250.0–377.6	–2.41559+1	4.20281+1	–1.59103+1	2.15754	V
115.4–250.0	1.08896+1	1.00531–1	7.99188–1	–6.11147–2	III
250.0–377.6	–1.31097+1	2.88997+1	–1.07205+1	1.47484	V

TABLE 11.7.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_p ($J K^{-1} g^{-1}$)	1.725	1.750	1.778	1.807	1.837	1.869	1.903
C_p ($J K^{-1} mol^{-1}$)	100.3	101.7	103.3	105.0	106.8	108.7	110.6
c_{sat} ($J K^{-1} g^{-1}$)	1.725	1.750	1.778	1.807	1.838	1.870	1.903
C_{sat} ($J K^{-1} mol^{-1}$)	100.2	101.7	103.3	105.0	106.8	108.7	110.6
Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1} g^{-1}$)	1.938	1.974	2.012	2.051	2.090	2.131	2.172
C_p ($J K^{-1} mol^{-1}$)	112.6	114.8	116.9	119.2	121.5	123.9	126.3
c_{sat} ($J K^{-1} g^{-1}$)	1.938	1.974	2.011	2.050	2.089	2.130	2.172
C_{sat} ($J K^{-1} mol^{-1}$)	112.6	114.7	116.9	119.1	121.4	123.8	126.2
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	2.22	2.26	2.28	2.31	2.37	2.42	2.43
C_p ($J K^{-1} mol^{-1}$)	129	131	132	134	138	141	141
c_{sat} ($J K^{-1} g^{-1}$)	2.21	2.26	2.27	2.31	2.36	2.41	2.42
C_{sat} ($J K^{-1} mol^{-1}$)	129	131	132	134	137	140	141
Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	2.50	2.59	2.69	2.81	2.94	3.09	3.26
C_p ($J K^{-1} mol^{-1}$)	146	151	156	163	171	180	190
c_{sat} ($J K^{-1} g^{-1}$)	2.49	2.56	2.65	2.74	2.85	2.98	3.11
C_{sat} ($J K^{-1} mol^{-1}$)	145	149	154	160	166	173	181
Temp. (K)	380						
c_p ($J K^{-1} g^{-1}$)	3.46						
C_p ($J K^{-1} mol^{-1}$)	201						
c_{sat} ($J K^{-1} g^{-1}$)	3.27						
C_{sat} ($J K^{-1} mol^{-1}$)	190						

TABLE 11.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	61	50	0.913	9.97–2	0.57	1.21–2	15
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
115.4–377.6	408.20	–2.42548	3.44901–1	9.38882	4.26424		V



Name: 2,2–Dimethylpropane
Formula: C_5H_{12}

CAS–RN: 463–82–1
Group No.: 11–008
Molar Mass: 72.15

TABLE 11.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36AST/MES	259.0–278.9	4	0.50	99.27	melpt	C_p	BSIO	36AST/MES
69ENO/SHI1	258.1–259.9	3	0.10	99.997	melpt	C_p	BSAO	66SHI/ATA

TABLE 11.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
36AST/MES	259.0–278.9	4	1.00#	0.984	1.86–1	0.98	–8.81–2	–2
69ENO/SHI1	258.0–259.9	3	0.30#	0.844	4.63–2	0.25	1.13–2	1

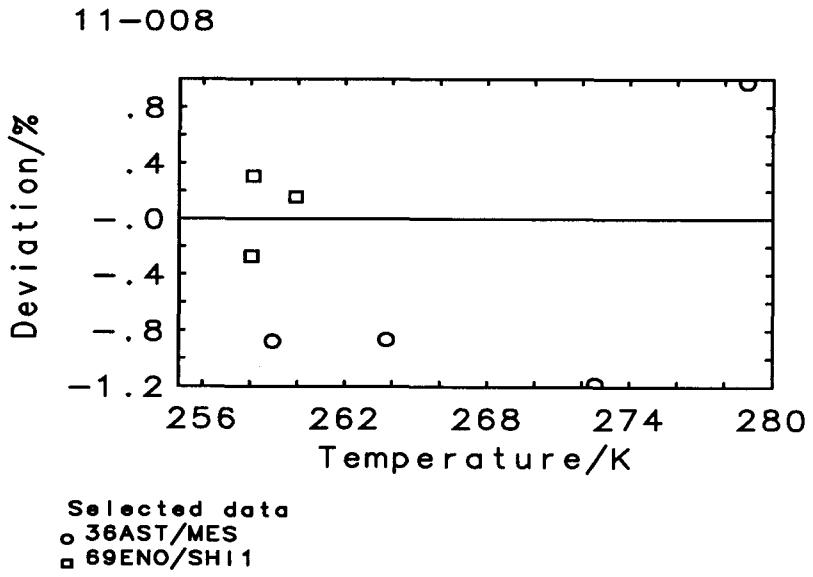
TABLE 11.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	1.096	1.70–1	0.90	–4.55–2	–1

Temp. range K	A_1	A_2	Level of uncertainty
258.0–278.9	2.84682	5.97751	IV

TABLE 11.8.4. Recommended values of heat capacities

Temp. (K)	260	265	270	273.15	275	280
c_p (J K^{-1}g^{-1})	2.119	2.153	2.188	2.210	2.222	2.257
C_p (J K^{-1}mol^{-1})	152.9	155.4	157.9	159.4	160.3	162.8



Name: 2-Methylbutane
Formula: C_5H_{12}

CAS-RN: 78-78-4
Group No.: 11-009
Molar Mass: 72.15

TABLE 11.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF2		120.5–275.8	14	1.00	not specified		C_p	BSIO	25PAR
42SCH/AST		120.0–290.0	13S	0.20	99.995	melpt	C_p	BSAO	39AST/EID1
43GUT/HUF	N	115.7–297.8	83	0.20	99.987	melpt	C_p	BSAO	43RUE/HUF
68SUG/ADA		113.4–298.3	88	nosp	99.986	melpt	C_{sat}	BSAO	65SUG/SEK
79VAN/ZEL2		120.0–270.0	16	nosp	99.9	anal	C_p	FSIO	79VAN/ZEL1
87CZA		289.0–298.3	3	1.00	not specified		C_p	BSIO	79CZA

43GUT/HUF smoothed values in 71MES/FIN

TABLE 11.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
43GUT/HUF	115.7–297.8	82	0.20	0.858	3.08–2	0.17	–2.42–2	–75
68SUG/ADA	113.4–298.3	87	0.20#	0.879	3.10–2	0.18	2.30–2	67
				Rejected data				
30PAR/HUF2	(8.71–2, 0.49, –6.76–2, –12)			42SCH/AST	(2.39–1, 1.21, 2.49–2, –7)			
79VAN/ZEL2	(1.45–1, 0.87, –1.40–1, –16)			87CZA	(1.02–1, 0.52, –1.01–1, –3)			

TABLE 11.9.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	217	169	0.882	3.14–2	0.18	1.07–4	–8

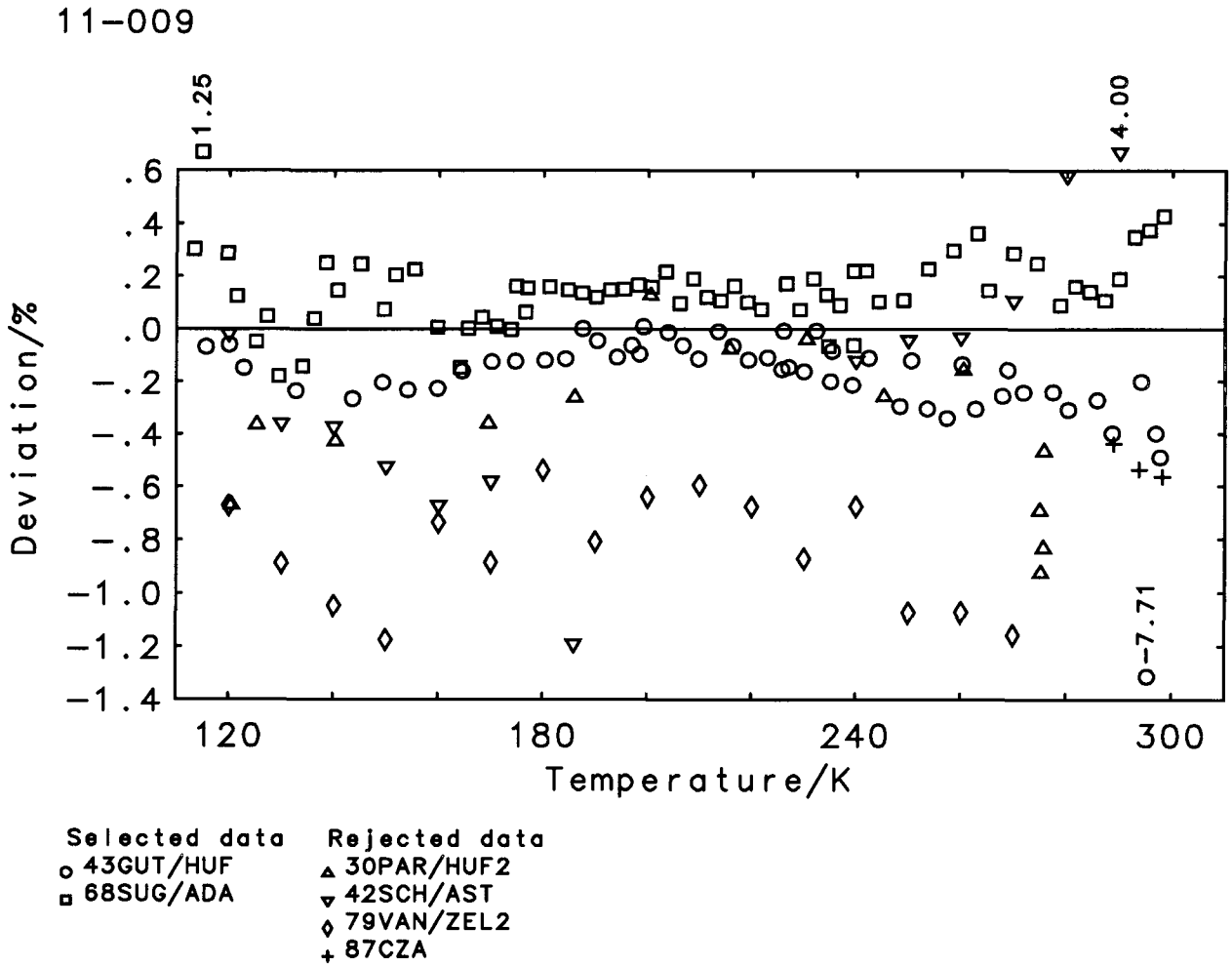
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
113.4–205.0	1.03413+1	6.50157	–3.03180	6.72000–1	II
205.0–298.3	1.77248+1	–4.30352	2.23898	–1.85037–1	II

TABLE 11.9.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c ($J K^{-1}g^{-1}$)	1.722	1.745	1.768	1.791	1.813	1.836	1.860
C ($J K^{-1}mol^{-1}$)	124.2	125.9	127.6	129.2	130.8	132.5	134.2
Temp. (K)	190	200	210	220	230	240	250
c ($J K^{-1}g^{-1}$)	1.885	1.912	1.942	1.973	2.007	2.044	2.082
C ($J K^{-1}mol^{-1}$)	136.0	138.0	140.1	142.4	144.8	147.5	150.2
Temp. (K)	260	270	273.15	280	290	298.15	300
c ($J K^{-1}g^{-1}$)	2.123	2.165	2.178	2.209	2.254	2.292	2.301
C ($J K^{-1}mol^{-1}$)	153.1	156.2	157.2	159.4	162.6	165.4	166.0

TABLE 11.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	217	169	1.081	3.85–2	0.22	1.55–4	–7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
113.4–298.3	460.40	–2.88905	1.59142	1.15863+1	1.31119		III



Name: Pentane
Formula: C_5H_{12}

CAS–RN: 109–66–0
Group No.: 11–010
Molar Mass: 72.15

TABLE 11.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
30PAR/HUF1		149.9–290.0	14	1.00	not specified	C_p	BSIO	25PAR
40MES/KEN		151.3–286.4	19	nosp	99.961 melpt	C_p	BSAO	39AST/EID1
67MES/GUT		148.6–302.9	25	0.20	99.86 melpt	C_{sat}	BSAO	47HUF
71AMI/ALI	N	313.1–468.1	19S	2.00	not specified	C_p	not specified	
75GRI/RAS	N	299.9–383.6	9	1.00	not specified	C_p	BDAO	75RAS/GRI
85CZA		299.0	1	nosp	not specified	C_p	BSIO	79CZA
88MEL/VER		153.1–433.1	10	2.50	not specified	C_{sat}	not specified	

71AMI/ALI calculated from Cv measured at the saturation line
75GRI/RAS all values (except the first one) at pressures above the vapour pressure

TABLE 11.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67MES/GUT	148.6–302.9	25	0.10	0.235	4.39–3	0.02	2.35–4	2
75GRI/RAS	299.9–383.6	9	1.00	0.527	1.16–1	0.53	–6.76–2	–5
88MEL/VER	153.1–393.1	9	2.50	0.200	1.10–1	0.50	2.76–2	1
				Rejected data				
30PAR/HUF1	(1.11–1, 0.60, –8.97–2, –12)			40MES/KEN	(1.28–1, 0.66, 2.25–2, –5)			
71AMI/ALI	(3.91–1, 1.78, 3.37–1, 9)			85CZA	(2.86–1, 1.44, –2.86–1, –1)			

TABLE 11.10.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	97	43	0.338	7.90–2	0.36	–8.23–3	–2
C_{sat}	97	43	0.311	7.50–2	0.34	–7.60–3	–3

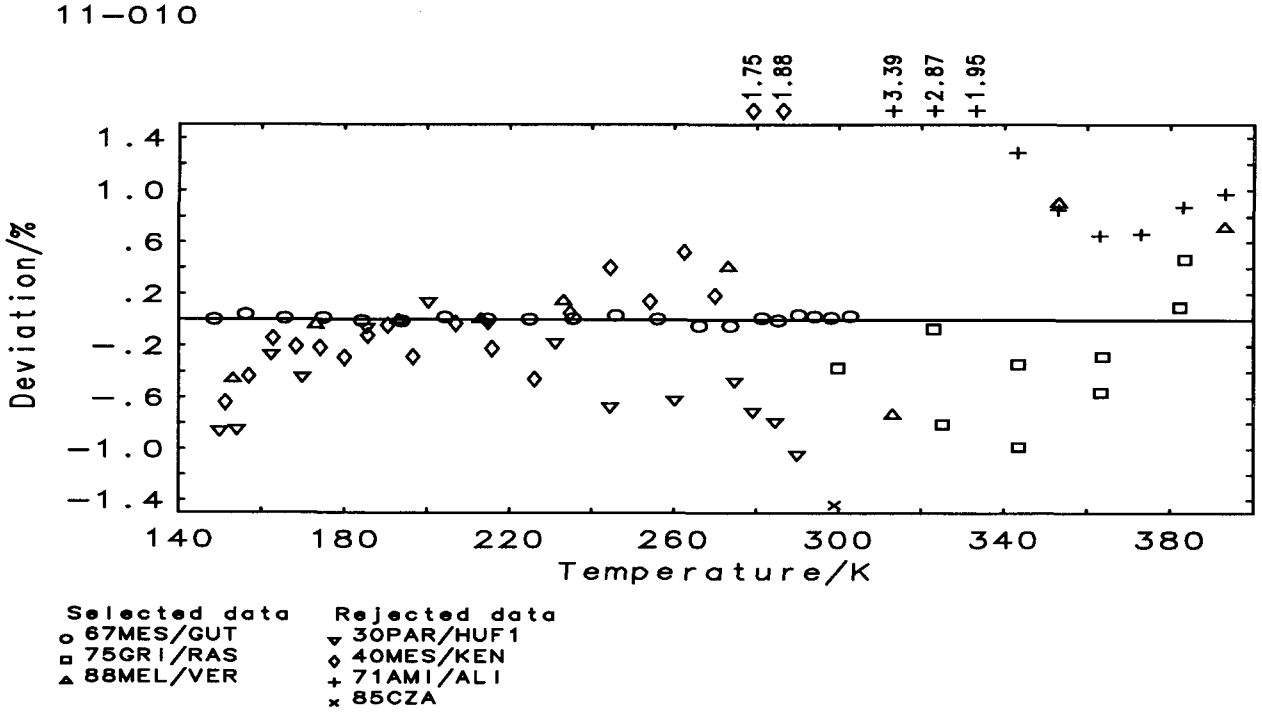
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
148.6–210.0	2.06484+1	–4.67090	1.47800	1.78866–2	II
210.0–290.0	2.35162+1	–8.76772	3.42886	–2.91773–1	II
290.0–393.1	1.33314+1	1.76823	–2.04216–1	1.25822–1	IV
148.6–210.0	2.04884+1	–4.40249	1.32945	4.49989–2	II
210.0–290.0	2.41030+1	–9.56614	3.78833	–3.45299–1	II
290.0–393.1	1.54904+1	–6.56541–1	7.16052–1	7.83648–3	IV

TABLE 11.10.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p ($J K^{-1}g^{-1}$)	1.962	1.963	1.967	1.974	1.986	2.001	2.019
C_p ($J K^{-1}mol^{-1}$)	141.6	141.6	141.9	142.5	143.3	144.4	145.7
c_{sat} ($J K^{-1}g^{-1}$)	1.962	1.963	1.967	1.974	1.986	2.001	2.019
C_{sat} ($J K^{-1}mol^{-1}$)	141.6	141.6	141.9	142.5	143.3	144.4	145.7
Temp. (K)	**220**	**230**	**240**	**250**	**260**	**270**	**273.15**
c_p ($J K^{-1}g^{-1}$)	2.042	2.067	2.096	2.128	2.163	2.201	2.213
C_p ($J K^{-1}mol^{-1}$)	147.3	149.2	151.2	153.6	156.1	158.8	159.7
c_{sat} ($J K^{-1}g^{-1}$)	2.042	2.067	2.096	2.128	2.163	2.200	2.213
C_{sat} ($J K^{-1}mol^{-1}$)	147.3	149.2	151.3	153.6	156.1	158.8	159.6
Temp. (K)	**280**	**290**	**298.15**	**300**	**310**	**320**	**330**
c_p ($J K^{-1}g^{-1}$)	2.241	2.283	2.319	2.327	2.374	2.422	2.474
C_p ($J K^{-1}mol^{-1}$)	161.7	164.7	167.3	167.9	171.3	174.8	178.5
c_{sat} ($J K^{-1}g^{-1}$)	2.240	2.282	2.317	2.325	2.370	2.418	2.466
C_{sat} ($J K^{-1}mol^{-1}$)	161.6	164.6	167.2	167.8	171.0	174.4	178.0
Temp. (K)	**340**	**350**	**360**	**370**	**380**	**390**	
c_p ($J K^{-1}g^{-1}$)	2.527	2.583	2.641	2.703	2.766	2.833	
C_p ($J K^{-1}mol^{-1}$)	182.3	186.4	190.6	195.0	199.6	204.4	
c_{sat} ($J K^{-1}g^{-1}$)	2.517	2.570	2.624	2.681	2.739	2.799	
C_{sat} ($J K^{-1}mol^{-1}$)	181.6	185.4	189.3	193.4	197.6	201.9	

TABLE 11.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	97	43	2.099	2.56–1	1.09	–2.45–3	–14
Temp. range K	**T_c K**	**A_1**	**A_2**	**A_3**	**A_4**	**A_5**	**A_6**	**Level of uncertainty**
148.6–393.1	469.80	5.13461+1	2.77849	1.31715+1	6.14601+1	–3.33298+1	1.00059+2	V



Name: 2,2–Dimethylbutane
Formula: C_6H_{14}

CAS–RN: 75–83–2
Group No.: 11–011
Molar Mass: 86.18

TABLE 11.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37STU	180.0–320.0	15S	nosp	not specified		C_p	BDHO	37STU
46DOU/HUF2	177.3–296.1	17	0.20	99.985	melpt	C_p	BSAO	43RUE/HUF
46KIL/PIT	178.7–279.6	12	0.20	99.995	melpt	C_p	BSAO	45GUT/PIT
50AUE/SAG	299.8–366.5	13	nosp	99.0	melpt	C_p	BSAO	39SAG/EVA
83BEN/DAR	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84BEN/DAR	298.1	1	nosp	99.88	estim	C_p	FSIT	71PIC/LED
86BEN/DAR1	298.1	1	nosp	99.88	anal	C_p	FSIT	71PIC/LED
88COS/VAN	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
89OHN/FUJ	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 11.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46DOU/HUF2	177.3–296.1	17	0.10	0.815	1.68–2	0.08	–4.75–3	–3
46KIL/PIT	178.7–279.6	12	0.20	0.922	3.93–2	0.18	2.02–2	4
50AUE/SAG	299.8–366.5	13	1.00#	0.619	1.47–1	0.62	9.69–2	5
83BEN/DAR	298.1	1	0.50#	0.000	3.81–5	0.00	–3.81–5	0
84BEN/DAR	298.1	1	0.50#	0.021	2.37–3	0.01	2.37–3	1
86BEN/DAR1	298.1	1	0.50#	0.316	3.60–2	0.16	3.60–2	1
89OHN/FUJ	298.1	1	0.30#	0.931	6.37–2	0.28	6.37–2	1
				Rejected data				
37STU	(7.00–1, 3.50, –6.22–1, –13)			88COS/VAN	(3.29–1, 1.43, 3.29–1, 1)			

TABLE 11.11.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	46	0.818	8.67–2	0.37	3.31–2	9
C_{sat}	62	46	0.936	8.63–2	0.37	3.32–2	11

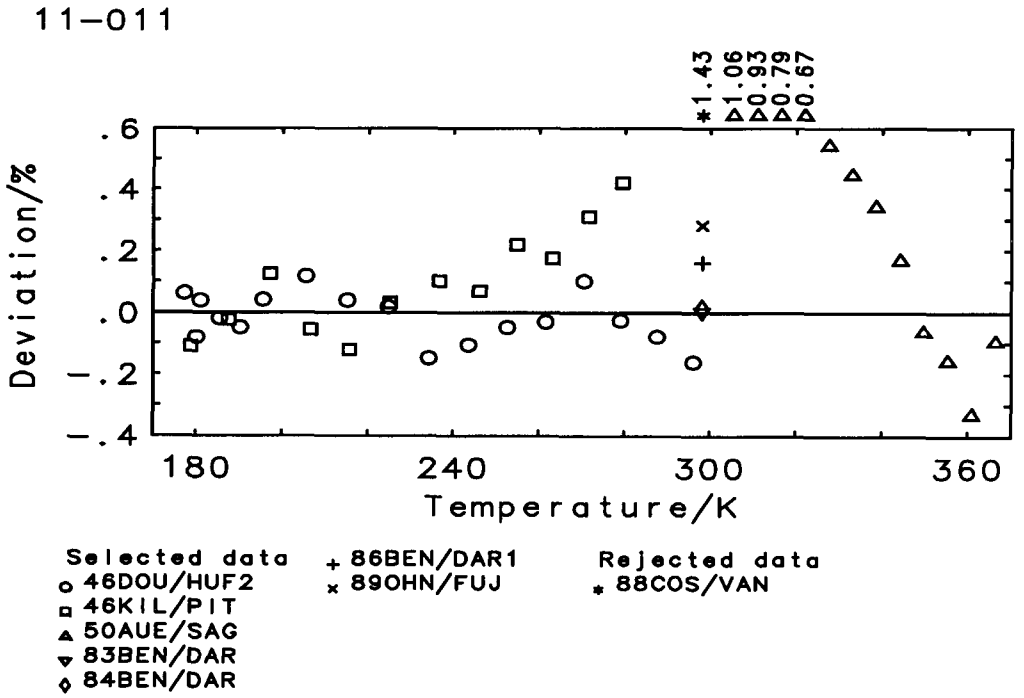
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
177.3–270.0	1.54212+1	1.56234–2	8.74132–1	–1.84652–2	II
270.0–366.5	1.59731+1	–5.97585–1	1.10125	–4.65041–2	IV
177.3–270.0	1.73539+1	–2.65154	2.08685	–2.00112–1	II
270.0–366.5	1.12115+1	4.17332	–4.40878–1	1.11954–1	IV

TABLE 11.11.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1} g^{-1}$)	1.753	1.783	1.814	1.846	1.880	1.916	1.953
C_p ($J K^{-1} mol^{-1}$)	151.1	153.7	156.3	159.1	162.0	165.1	168.3
c_{sat} ($J K^{-1} g^{-1}$)	1.754	1.783	1.814	1.846	1.880	1.916	1.953
C_{sat} ($J K^{-1} mol^{-1}$)	151.1	153.6	156.3	159.1	162.1	165.1	168.3
Temp. (K)	**250**	**260**	**270**	**273.15**	**280**	**290**	**298.15**
c_p ($J K^{-1} g^{-1}$)	1.991	2.031	2.072	2.085	2.114	2.158	2.195
C_p ($J K^{-1} mol^{-1}$)	171.6	175.0	178.5	179.7	182.2	186.0	189.1
c_{sat} ($J K^{-1} g^{-1}$)	1.991	2.031	2.071	2.084	2.113	2.155	2.190
C_{sat} ($J K^{-1} mol^{-1}$)	171.6	175.0	178.5	179.6	182.1	185.7	188.8
Temp. (K)	**300**	**310**	**320**	**330**	**340**	**350**	**360**
c_p ($J K^{-1} g^{-1}$)	2.203	2.250	2.298	2.347	2.397	2.449	2.501
C_p ($J K^{-1} mol^{-1}$)	189.9	193.9	198.0	202.2	206.6	211.0	215.5
c_{sat} ($J K^{-1} g^{-1}$)	2.198	2.243	2.289	2.335	2.384	2.433	2.484
C_{sat} ($J K^{-1} mol^{-1}$)	189.5	193.3	197.2	201.3	205.4	209.7	214.1

TABLE 11.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	46	1.403	1.32–1	0.56	5.52–2	12
Temp. range K	**T_c K**	**A_1**	**A_2**	**A_3**	**A_4**		**Level of uncertainty**
177.3–366.5	488.80	–4.16296	5.24633–1	1.23638+1	8.25827		IV



Name: 2,3–Dimethylbutane
Formula: C_6H_{14}

CAS–RN: 79–29–8
Group No.: 11–012
Molar Mass: 86.18

TABLE 11.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37STU	140.0–320.0	19S	nosp	not specified		C_p	BDHO	37STU
46DOU/HUF2	149.4–306.5	38	0.20	99.985	melpt	C_p	BSAO	43RUE/HUF
71ADA/SUG	146.9–302.9	48	nosp	99.87	melpt	C_p	BSAO	65SUG/SEK
82WIL/FAR	298.1	1	nosp	99.	estim	C_p	FSIT	71PIC/LED
83BEN/DAR	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84BEN/DAR	298.1	1	nosp	99.98	melpt	C_p	FSIT	71PIC/LED
84FIL/LAU	293.0	1	2.00	98.	anal	C_p	BDHO	84FIL/LAU
86BEN/DAR1	298.1	1	nosp	99.88	anal	C_p	FSIT	71PIC/LED
89OHN/FUJ	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 11.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46DOU/HUF2	149.4–306.5	38	0.20#	1.045	4.23–2	0.21	–3.18–2	–29
71ADA/SUG	146.9–302.9	48	0.20#	1.020	4.41–2	0.20	2.59–2	41
82WIL/FAR	298.1	1	0.50#	0.283	3.21–2	0.14	–3.21–2	–1
83BEN/DAR	298.1	1	0.50#	0.315	3.57–2	0.16	–3.57–2	–1
84BEN/DAR	298.1	1	0.50#	0.421	4.78–2	0.21	–4.78–2	–1
86BEN/DAR1	298.1	1	0.50#	0.029	3.26–3	0.01	–3.26–3	–1
89OHN/FUJ	298.1	1	0.30#	0.083	5.67–3	0.02	–5.67–3	–1
				Rejected data				
37STU	(8.09–1, 4.07, 5.42–1, 8)			84FIL/LAU	(1.14–1, 0.51, –1.14–1, –1)			

TABLE 11.12.3. Parameters of regression polynomial

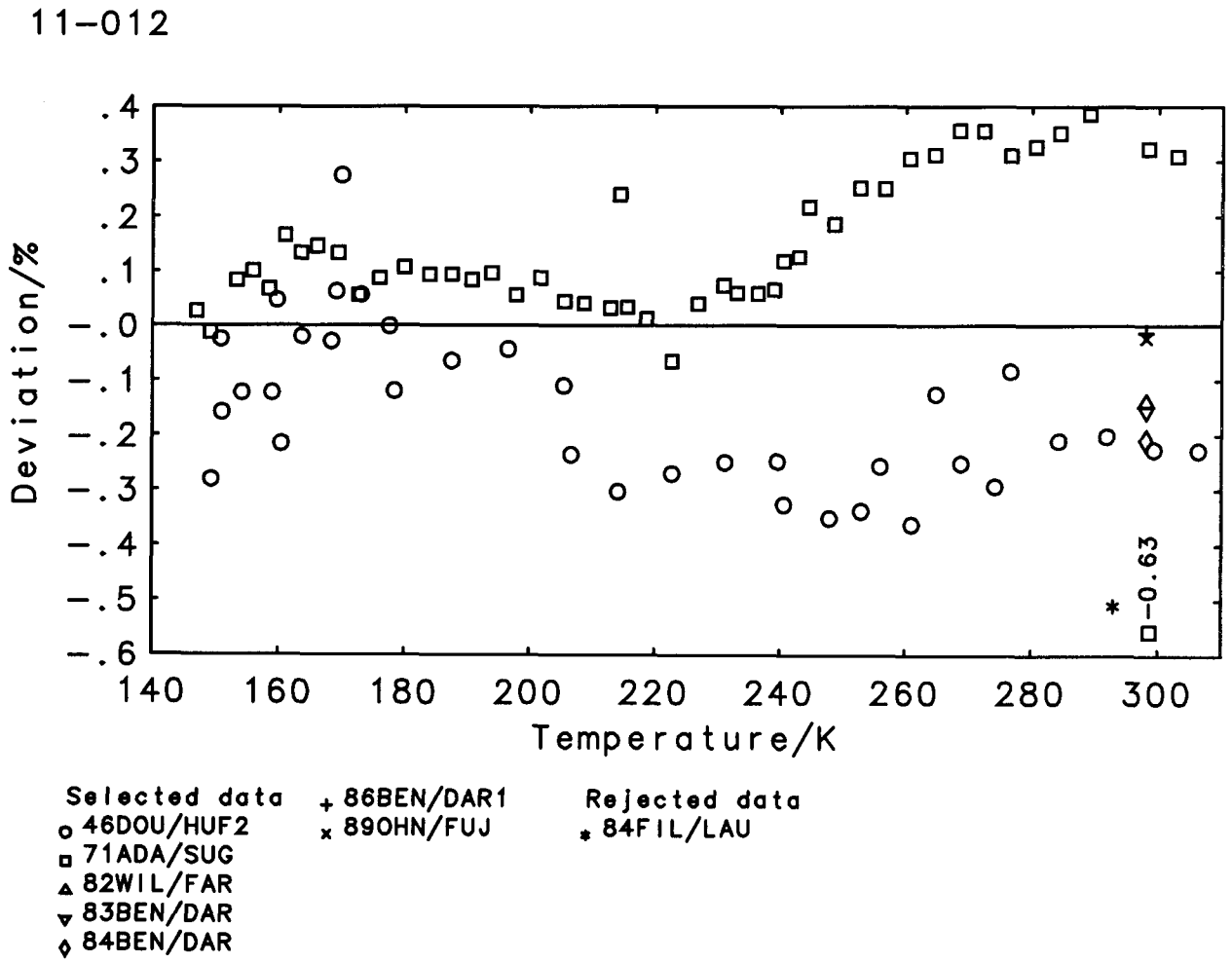
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	111	91	1.027	4.37–2	0.21	–9.64–4	7
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
146.9–306.5	1.46648+1	1.50058	1.57352–1	8.30773–2			II

TABLE 11.12.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p ($J K^{-1}g^{-1}$)	1.693	1.718	1.744	1.771	1.800	1.829	1.860
C_p ($J K^{-1}mol^{-1}$)	145.9	148.1	150.3	152.7	155.1	157.6	160.3
Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J K^{-1}g^{-1}$)	1.892	1.926	1.961	1.997	2.035	2.074	2.087
C_p ($J K^{-1}mol^{-1}$)	163.1	166.0	169.0	172.1	175.4	178.8	179.8
Temp. (K)	280	290	298.15	300	310		
c_p ($J K^{-1}g^{-1}$)	2.115	2.158	2.194	2.202	2.248		
C_p ($J K^{-1}mol^{-1}$)	182.3	186.0	189.1	189.8	193.8		

TABLE 11.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	111	91	1.075	4.64–2	0.22	–1.91–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
146.9–306.5	500.00	–4.66092	1.52954	1.26220+1	3.55076		II



Name: Hexane
Formula: C_6H_{14}

CAS–RN: 110–54–3
Group No.: 11–013
Molar Mass: 86.18

TABLE 11.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF2		183.5–295.1	8	nosp	not specified		C_p	BSIO	25PAR
31HUF/PAR		188.8–293.5	5	1.00	not specified		C_p	BSIO	25PAR
37STU		180.0–320.0	15S	nosp	not specified		C_p	BDHO	37STU
39PHI		300.6	1	nosp	not specified		C_p	BSIO	49WEI
46DOU/HUF2	N	180.4–301.0	24	0.20	99.992	melpt	C_p	BSAO	43RUE/HUF
51CON/SAG		299.8–366.5	13S	0.70	not specified		C_p	BSAO	39SAG/EVA
69WIL/ROT		293.1	1	0.40	not specified		C_p	BDAO	65FIN/GRU
71AMI/ALI	N	343.1–506.1	19S	2.00	not specified		C_p	not specified	
71REC/SAD		303.1	1	0.30	not specified		C_p	BSIO	70REC
74DIA/REN		298.2–324.7	14	0.30	not specified		C_p	BSAO	74DIA/REN
75GRI/RAS	N	304.5–463.1	9	1.00	not specified		C_p	BDAO	75RAS/GRI
76KAR/GRO		298.2	1	nosp	not specified		C_p	FSIT	71PIC/LED
80KAL/JED		180.6–301.4	33	0.20	99.95	chrom	C_p	BSAO	80KAL/JED
81GRO/ING		298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED
82WIL/ING		298.1	1	nosp	99.5	estim	C_p	FSIT	71PIC/LED
84BEN/DAR		298.1	1	nosp	99.98	melpt	C_p	FSIT	71PIC/LED
84BRA/PIN		298.1	1	nosp	99.0	melpt	C_p	FSIT	71PIC/LED
85COS/PAT1		298.2	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
85COS/PAT8		298.1–313.1	2	nosp	99.	estim	C_p	FSIT	71PIC/LED
85CZA		299.9	1	nosp	not specified		C_p	BSIO	79CZA
86BEN/DAR1		298.1	1	nosp	99.88	anal	C_p	FSIT	71PIC/LED
86NAZ/BAS2		308.4–333.1	2	2.00	99.8	estim	C_p	BDHO	86NAZ/BAS1
88MEL/VER		183.1–473.1	11	2.50	not specified		C_{sat}	not specified	
88SAI/TAN		298.1	1	nosp	99.95	anal	C_p	FSIT	71PIC/LED
89OHN/FUJ		298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA
89VOG/SCH		333.1	1	nosp	not specified		C_p	BDHT	69PER/COM
91OGA/MIT		298.1	1	nosp	not specified		C_p	FSIO	85OGA
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

46DOU/HUF2 smoothed data in 67MES/GUT
71AMI/ALI calculated from Cv measured at the saturation line
75GRI/RAS all values (except the first one) at pressures above the vapour pressure

TABLE 11.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31HUF/PAR	188.8–293.5	5	1.00	0.242	5.46–2	0.24	–3.68–2	–1
46DOU/HUF2	180.4–301.0	24	0.20#	0.589	2.48–2	0.12	–2.99–3	–1
51CON/SAG	299.8–366.5	13	0.70	0.382	6.90–2	0.27	5.70–2	9
69WIL/ROT	293.1	1	0.40	1.053	9.78–2	0.42	–9.78–2	–1
75GRI/RAS	304.5–463.1	9	1.00	0.631	1.88–1	0.63	–3.49–2	–1
76KAR/GRO	298.2	1	0.50#	0.457	5.39–2	0.23	5.39–2	1
80KAL/JED	180.6–301.4	33	0.20	1.125	4.81–2	0.23	2.74–3	–1
81GRO/ING	298.1	1	0.50#	0.005	6.26–4	0.00	6.26–4	0
82WIL/ING	298.1	1	0.50#	0.343	4.03–2	0.17	–4.03–2	–1
84BEN/DAR	298.1	1	0.50#	0.138	1.63–2	0.07	1.63–2	1
84BRA/PIN	298.1	1	0.50#	0.343	4.03–2	0.17	–4.03–2	–1
86BEN/DAR1	298.1	1	0.50#	0.179	2.11–2	0.09	2.11–2	1
88MEL/VER	183.1–413.1	10	2.50	0.137	8.13–2	0.34	–3.73–2	–4
88SAI/TAN	298.1	1	0.50#	0.025	2.98–3	0.01	–2.98–3	–1
89OHN/FUJ	298.1	1	0.30#	0.760	5.35–2	0.23	–5.35–2	–1

	Rejected data		
30PAR/HUF2	(2.39–1, 1.08, –2.19–1, –8)	37STU	(1.24, 5.21, 6.35–1, 4)
39PHI	(1.26, 5.64, –1.26, –1)	71AMI/ALI	(5.45–1, 1.89, –3.33–1, –5)
71REC/SAD	(3.04–1, 1.30, –3.04–1, –1)	74DIA/REN	(6.32–1, 2.50, 5.70–1, 14)
85COS/PAT1	(2.38–1, 1.00, 2.38–1, 1)	85COS/PAT8	(2.88–1, 1.17, 1.57–1, 0)
85CZA	(1.80–1, 0.77, –1.80–1, –1)	86NAZ/BAS2	(5.19–1, 2.06, 5.15–1, 2)
89VOG/SCH	(8.22–1, 3.16, 8.22–1, 1)	91OGA/MIT	(1.46–1, 0.62, 1.46–1, 1)
91TRE/COS	(2.40–1, 1.01, 2.40–1, 1)		

TABLE 11.13.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	171	103	0.775	7.67–2	0.29	–2.47–3	–1
C_{sat}	171	103	0.764	6.78–2	0.27	–2.69–3	3

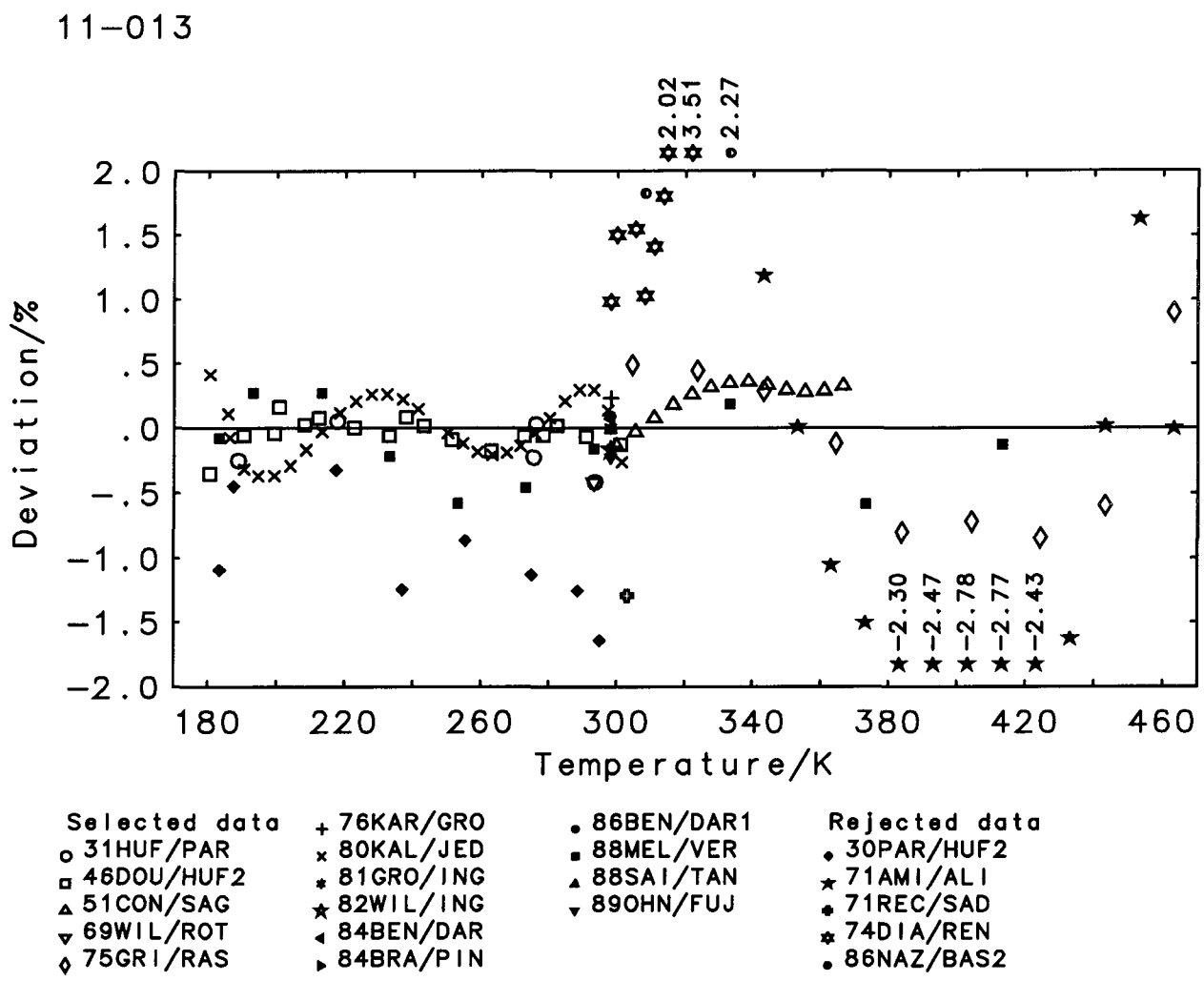
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
180.4–250.0	4.62532+1	–3.38510+1	1.40593+1	–1.77381	II
250.0–330.0	1.25487+1	6.59447	–2.11887	3.83276–1	III
330.0–463.1	5.66582+1	–3.35051+1	1.00325+1	–8.44136–1	IV
180.4–250.0	4.63534+1	–3.39839+1	1.41172+1	–1.78209	II
250.0–330.0	1.28287+1	6.24568	–1.97461	3.63490–1	III
330.0–463.1	6.93905+1	–4.51742+1	1.36072+1	–1.21043	IV

TABLE 11.13.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.981	1.980	1.987	2.001	2.020	2.044	2.072
C_p (J K^{-1}mol^{-1})	170.7	170.6	171.3	172.4	174.1	176.2	178.5
c_{sat} (J K^{-1}g^{-1})	1.981	1.980	1.987	2.001	2.020	2.044	2.072
C_{sat} (J K^{-1}mol^{-1})	170.7	170.6	171.3	172.4	174.1	176.2	178.5
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.101	2.133	2.166	2.177	2.201	2.238	2.270
C_p (J K^{-1}mol^{-1})	181.1	183.8	186.7	187.6	189.7	192.9	195.7
c_{sat} (J K^{-1}g^{-1})	2.101	2.133	2.166	2.177	2.201	2.238	2.270
C_{sat} (J K^{-1}mol^{-1})	181.1	183.8	186.7	187.6	189.7	192.9	195.6
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.278	2.320	2.365	2.413	2.464	2.518	2.574
C_p (J K^{-1}mol^{-1})	196.3	199.9	203.8	207.9	212.3	217.0	221.8
c_{sat} (J K^{-1}g^{-1})	2.278	2.320	2.364	2.412	2.462	2.515	2.570
C_{sat} (J K^{-1}mol^{-1})	196.3	199.9	203.8	207.9	212.2	216.8	221.5
Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.632	2.691	2.751	2.811	2.871	2.930	2.988
C_p (J K^{-1}mol^{-1})	226.8	231.9	237.0	242.2	247.4	252.5	257.5
c_{sat} (J K^{-1}g^{-1})	2.626	2.682	2.738	2.792	2.845	2.896	2.943
C_{sat} (J K^{-1}mol^{-1})	226.3	231.1	235.9	240.6	245.2	249.5	253.6
Temp. (K)	440	450	460				
c_p (J K^{-1}g^{-1})	3.045	3.099	3.151				
C_p (J K^{-1}mol^{-1})	262.4	267.1	271.5				
c_{sat} (J K^{-1}g^{-1})	2.986	3.025	3.058				
C_{sat} (J K^{-1}mol^{-1})	257.3	260.7	263.6				

TABLE 11.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	171	102	3.699	3.17–1	1.27	6.79–2	–8
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
180.4–443.1	507.90	–3.44495	4.67981–1	1.56153+1	6.33982		V



Name: 2–Methylpentane
Formula: C_6H_{14}

CAS–RN: 107–83–5
Group No.: 11–014
Molar Mass: 86.18

TABLE 11.14.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
37STU		120.0–320.0	21S	nosp	not specified		C_p	BDHO	37STU
46DOU/HUF2	N	117.4–303.3	28	0.20	99.971	melpt	C_p	BSAO	43RUE/HUF
83BEN/DAR		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84BEN/DAR		298.1	1	nosp	99.98	melpt	C_p	FSIT	71PIC/LED
84FIL/LAU		293.0	1	2.00	97.	anal	C_p	BDHO	84FIL/LAU
86BEN/DAR1		298.1	1	nosp	99.88	anal	C_p	FSIT	71PIC/LED
89OHN/FUJ		298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

46DOU/HUF2 smoothed values in 71MES/FIN

TABLE 11.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46DOU/HUF2	117.4–303.3	28	0.20	0.411	1.57–2	0.08	–3.61–4	2
83BEN/DAR	298.1	1	0.50#	0.132	1.53–2	0.07	1.53–2	1
84BEN/DAR	298.1	1	0.50#	0.214	2.50–2	0.11	2.50–2	1
86BEN/DAR1	298.1	1	0.50#	0.255	2.98–2	0.13	2.98–2	1
				Rejected data				
37STU	(7.01–1, 3.28, 5.78–1, 13)			84FIL/LAU	(8.35–1, 3.76, –8.35–1, –1)			
89OHN/FUJ	(5.74–2, 0.25, 5.74–2, 1)							

TABLE 11.14.3. Parameters of regression polynomial

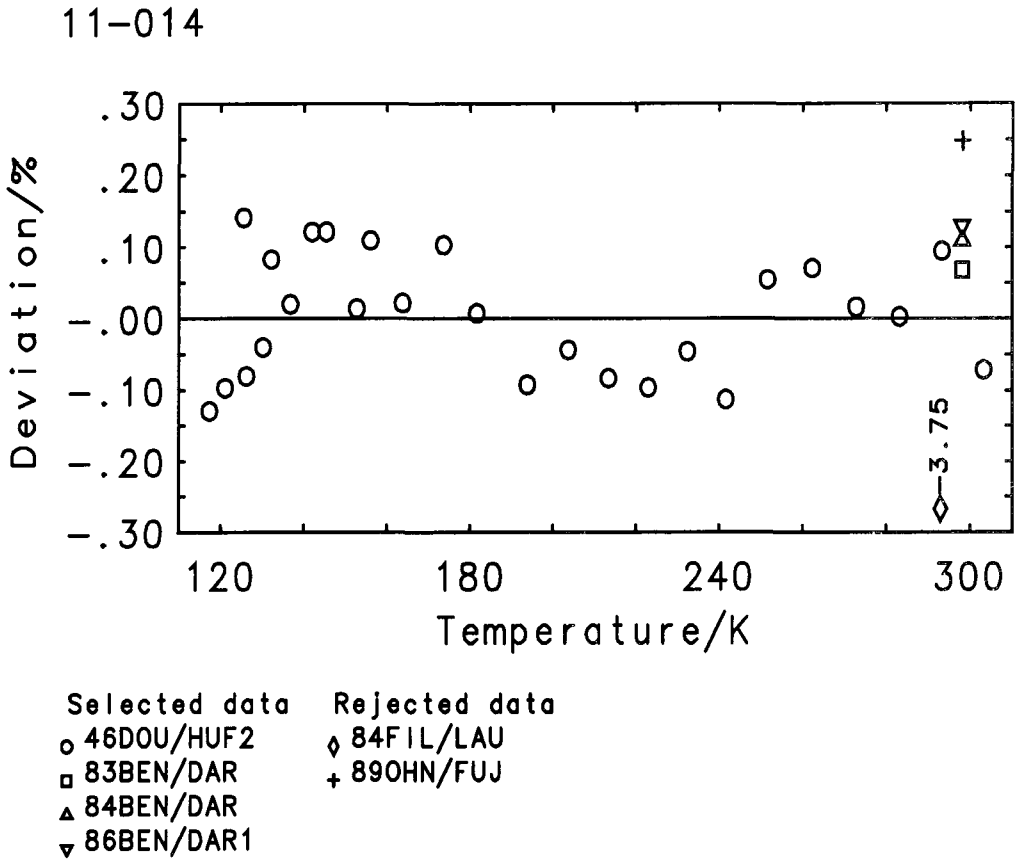
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	54	31	0.417	1.76–2	0.09	1.93–3	5
Temp. range K	A_1	A_2	A_3				Level of uncertainty
117.4–303.3	1.71510+1	–6.17987–1	8.98789–1				II

TABLE 11.14.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_p (J K^{-1}g^{-1})	1.708	1.724	1.741	1.760	1.781	1.804	1.828
C_p (J K^{-1}mol^{-1})	147.2	148.6	150.1	151.7	153.5	155.5	157.6
Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.855	1.882	1.912	1.943	1.976	2.011	2.048
C_p (J K^{-1}mol^{-1})	159.8	162.2	164.8	167.5	170.3	173.3	176.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.086	2.126	2.139	2.168	2.211	2.248	2.256
C_p (J K^{-1}mol^{-1})	179.8	183.2	184.3	186.8	190.5	193.7	194.4

TABLE 11.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	54	31	0.968	4.46–2	0.21	–6.52–3	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
117.4–303.3	497.50	–2.53223	3.33295	1.24549+1	4.80969–1		II



Name: 3-Methylpentane
Formula: C_6H_{14}

CAS-RN: 96-14-0
Group No.: 11-015
Molar Mass: 86.18

TABLE 11.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37STU	120.0–320.0	21S	3.00	not specified		C_p	BDHO	37STU
46DOU/HUF2	125.3–302.1	19	0.20	not specified		C_p	BSAO	43RUE/HUF
73FIN/MES	119.0–327.3	24	0.20	99.994	melpt	C_{sat}	BSAO	43RUE/HUF
80CZA	298.9	1	nosp	not specified		C_p	BSIO	79CZA
82OGU/WAT	119.5–288.2	64	1.00	not specified		C_p	BSAO	82OGU/WAT
83BEN/DAR	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84BEN/DAR	298.1	1	0.20	99.98	chrom	C_p	FSIT	71PIC/LED
84FIL/LAU	293.0	1	2.00	99.	anal	C_p	BDHO	84FIL/LAU
86BEN/DAR1	298.1	1	nosp	99.88	anal	C_p	FSIT	71PIC/LED
89OHN/FUJ	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 11.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
46DOU/HUF2	125.3–302.1	19	0.20	0.541	2.09–2	0.11	−1.04–3	0
73FIN/MES	119.1–327.3	24	0.20	0.246	1.03–2	0.05	−1.61–3	−1
83BEN/DAR	298.1	1	0.50#	0.118	1.36–2	0.06	1.36–2	1
84BEN/DAR	298.1	1	0.20	0.532	2.44–2	0.11	2.44–2	1
86BEN/DAR1	298.1	1	0.50#	0.349	4.00–2	0.17	4.00–2	1
89OHN/FUJ	298.1	1	0.30#	0.877	6.05–2	0.26	6.05–2	1
				Rejected data				
37STU	(7.11–1, 3.56, 5.15–1, 13)			80CZA	(5.03–1, 2.24, −5.03–1, −1)			
82OGU/WAT	(9.09–2, 0.46, 4.86–2, 34)			84FIL/LAU	(9.01–2, 0.40, 9.01–2, 1)			

TABLE 11.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	134	47	0.432	1.96–2	0.09	1.71–3	3
Temp. range K	A_1	A_2	A_3				Level of uncertainty
119.1–327.3	1.69688+1	−4.86827–1	8.33953–1				II

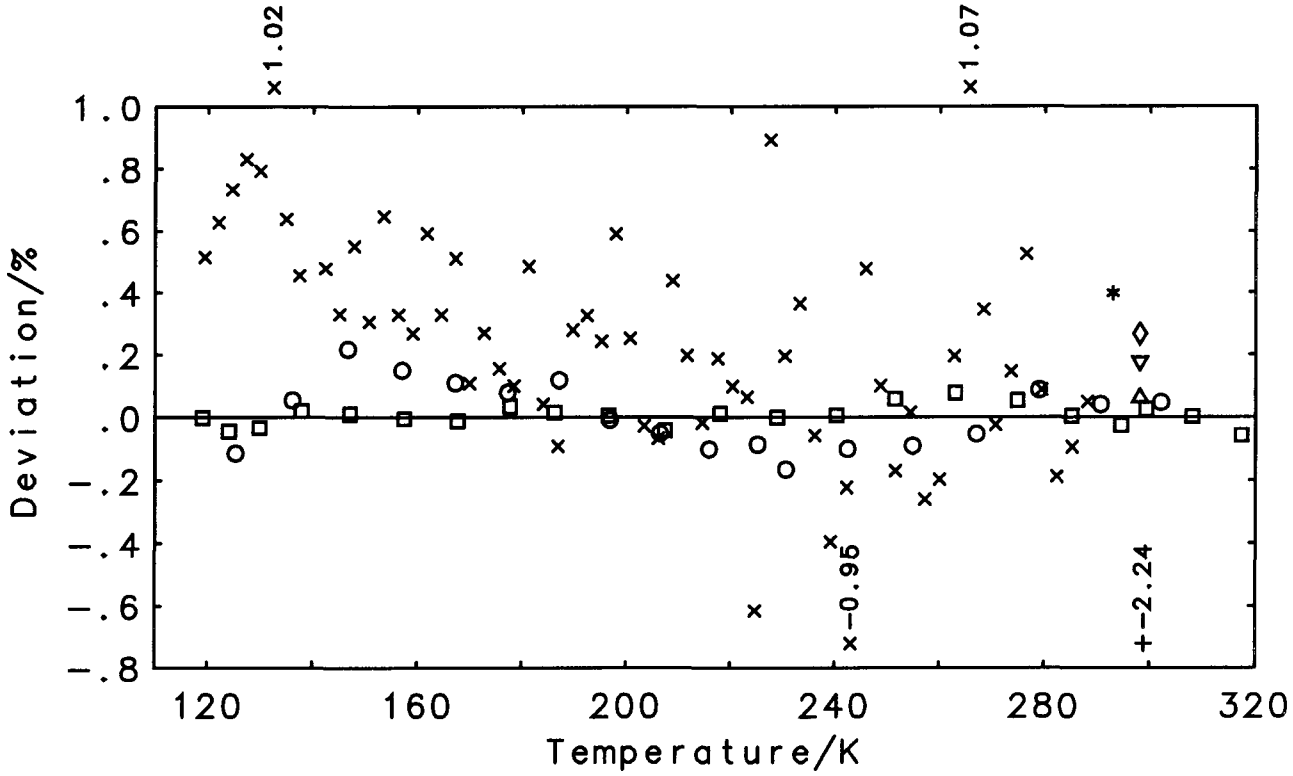
TABLE 11.15.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c ($J K^{-1} g^{-1}$)	1.697	1.712	1.729	1.748	1.768	1.790	1.813
C ($J K^{-1} mol^{-1}$)	146.2	147.5	149.0	150.6	152.4	154.2	156.3
Temp. (K)	190	200	210	220	230	240	250
c ($J K^{-1} g^{-1}$)	1.838	1.865	1.893	1.923	1.955	1.988	2.023
C ($J K^{-1} mol^{-1}$)	158.4	160.7	163.2	165.7	168.5	171.3	174.3
Temp. (K)	260	270	273.15	280	290	298.15	300
c ($J K^{-1} g^{-1}$)	2.059	2.097	2.109	2.136	2.178	2.212	2.220
C ($J K^{-1} mol^{-1}$)	177.4	180.7	181.8	184.1	187.7	190.7	191.3
Temp. (K)	310	320	330				
c ($J K^{-1} g^{-1}$)	2.265	2.311	2.358				
C ($J K^{-1} mol^{-1}$)	195.2	199.1	203.2				

TABLE 11.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	134	47	1.343	6.08–2	0.27	−7.69–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
119.1–327.3	504.50	−3.36575	2.60533	1.29200+1	1.08703		II

11–015



Selected data
- o 46DOU/HUF2
- □ 73FIN/MES
- △ 83BEN/DAR
- ▽ 86BEN/DAR1
- ◇ 89OHN/FUJ

Rejected data
- + 80CZA
- × 82OGU/WAT
- * 84FIL/LAU

Name: 2,2–Dimethylpentane
Formula: C_7H_{16}

CAS–RN: 590–35–2
Group No.: 11–016
Molar Mass: 100.20

TABLE 11.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30HUF/PAR2	153.2–294.1	14	1.00	not specified		C_p	BSIO	25PAR
61HUF/GRO	154.7–298.4	20	0.20	99.83	melpt	C_{sat}	BSAO	47HUF

TABLE 11.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61HUF/GRO	154.7298.4	20	0.20#	0.141	6.82–3	0.03	–1.91–7	0
				Rejected data				
30HUF/PAR2	(2.04–1, 0.88, –1.94–1, –12)							

TABLE 11.16.3. Parameters of regression polynomial

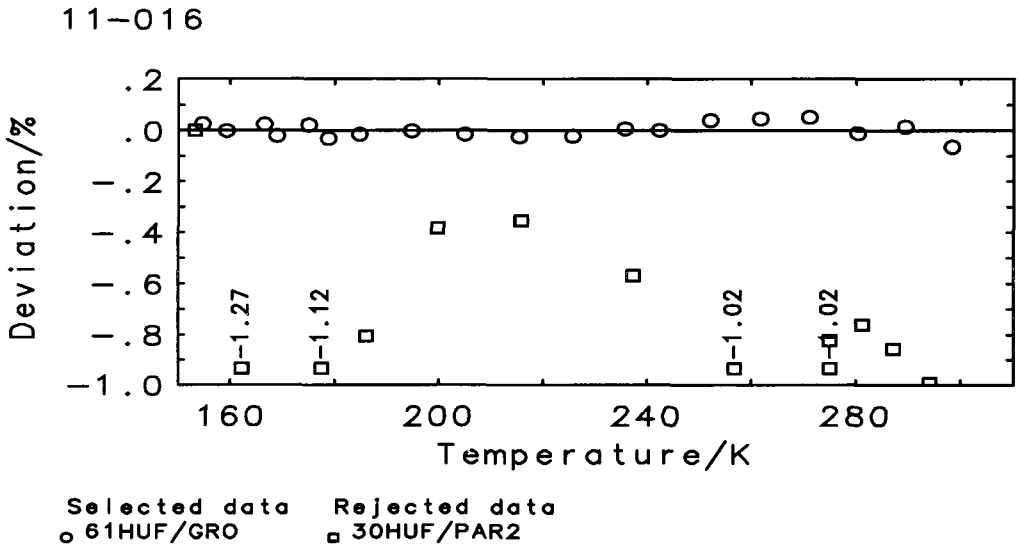
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	20	0.153	7.39–3	0.03	–1.91–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
154.7–298.4		1.62607+1	1.14508	7.80583–1			II

TABLE 11.16.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.667	1.698	1.730	1.764	1.798	1.834	1.872
C_{sat} (J K^{-1}mol^{-1})	167.0	170.1	173.4	176.7	180.2	183.8	187.6
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.910	1.950	1.992	2.034	2.078	2.092	2.123
C_{sat} (J K^{-1}mol^{-1})	191.4	195.4	199.6	203.8	208.2	209.6	212.7
Temp. (K)	290	298.15	300				
c_{sat} (J K^{-1}g^{-1})	2.169	2.208	2.217				
C_{sat} (J K^{-1}mol^{-1})	217.4	221.3	222.2				

TABLE 11.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	20	0.458	2.15–2	0.09	3.34–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
154.7–298.4	520.50	–6.75415	1.76171	1.30664+1	6.47362		II



Name: 2,3–Dimethylpentane
Formula: C_7H_{16}

CAS–RN: 565–59–3
Group No.: 11–017
Molar Mass: 100.20

TABLE 11.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30HUF/PAR2	90.4–291.3	15	1.00	not specified		C_p	BSIO	25PAR
76FIN/MES	84.0–385.3	69	0.20	99.8	estim	C_{sat}	BSAO	43RUE/HUF
84FIL/LAU	293.0	1	2.00	95.	anal	C_p	BDHO	84FIL/LAU

TABLE 11.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76FIN/MES	85.0–385.3	68	0.20	1.009	4.39–2	0.20	1.46–4	4
				Rejected data				
30HUF/PAR2	(7.25–2, 0.31, –5.06–2, –6)			84FIL/LAU	(6.09–1, 2.41, –6.09–1, –1)			

TABLE 11.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	85	68	1.032	4.49–2	0.21	1.46–4	4
C_{sat}	85	68	1.069	4.78–2	0.21	1.43–4	4

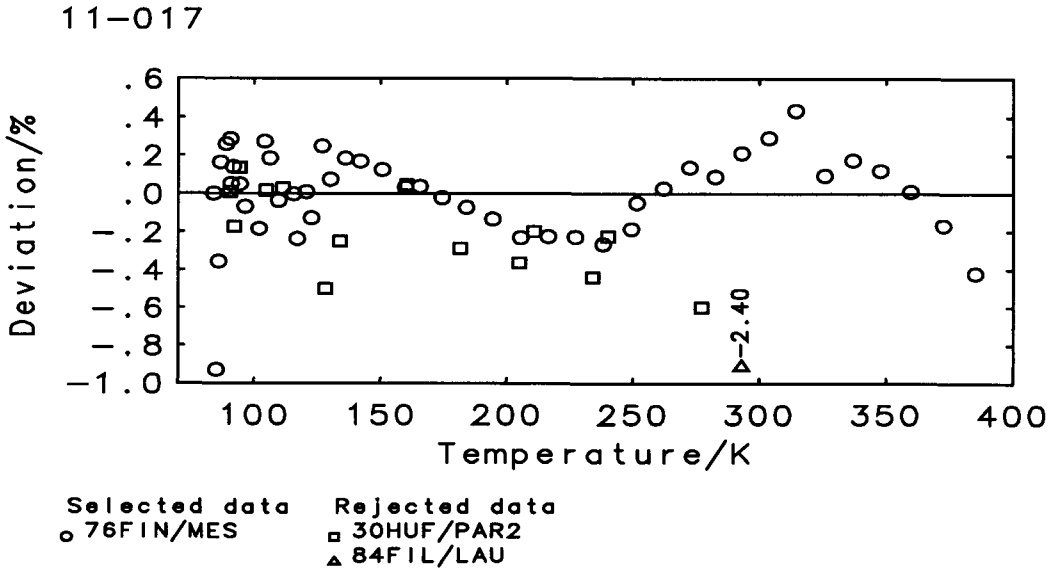
Temp. range K	A_1	A_2	A_3	Level of uncertainty
85.0–385.3	1.76512+1	6.68788–1	7.36103–1	II
85.0–385.3	1.76323+1	6.95008–1	7.28393–1	II

TABLE 11.17.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_p ($J\,K^{-1}g^{-1}$)	1.564	1.581	1.600	1.619	1.640	1.662	1.685
C_p ($J\,K^{-1}mol^{-1}$)	156.7	158.4	160.3	162.2	164.3	166.5	168.9
c_{sat} ($J\,K^{-1}g^{-1}$)	1.564	1.581	1.600	1.619	1.640	1.662	1.686
C_{sat} ($J\,K^{-1}mol^{-1}$)	156.7	158.4	160.3	162.3	164.4	166.6	168.9
Temp. (K)	160	170	180	190	200	210	220
c_p ($J\,K^{-1}g^{-1}$)	1.710	1.735	1.762	1.791	1.820	1.851	1.882
C_p ($J\,K^{-1}mol^{-1}$)	171.3	173.9	176.6	179.4	182.4	185.4	188.6
c_{sat} ($J\,K^{-1}g^{-1}$)	1.710	1.736	1.763	1.791	1.820	1.851	1.882
C_{sat} ($J\,K^{-1}mol^{-1}$)	171.4	173.9	176.6	179.4	182.4	185.4	188.6
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	1.915	1.950	1.985	2.022	2.060	2.072	2.099
C_p ($J\,K^{-1}mol^{-1}$)	191.9	195.4	198.9	202.6	206.4	207.6	210.3
c_{sat} ($J\,K^{-1}g^{-1}$)	1.915	1.950	1.985	2.022	2.059	2.072	2.098
C_{sat} ($J\,K^{-1}mol^{-1}$)	191.9	195.4	198.9	202.6	206.4	207.6	210.3
Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	2.139	2.173	2.181	2.224	2.268	2.313	2.359
C_p ($J\,K^{-1}mol^{-1}$)	214.4	217.7	218.5	222.8	227.2	231.8	236.4
c_{sat} ($J\,K^{-1}g^{-1}$)	2.139	2.172	2.180	2.223	2.266	2.312	2.358
C_{sat} ($J\,K^{-1}mol^{-1}$)	214.3	217.7	218.4	222.7	227.1	231.6	236.3
Temp. (K)	350	360	370	380	390		
c_p ($J\,K^{-1}g^{-1}$)	2.407	2.456	2.506	2.557	2.610		
C_p ($J\,K^{-1}mol^{-1}$)	241.2	246.1	251.1	256.3	261.5		
c_{sat} ($J\,K^{-1}g^{-1}$)	2.405	2.454	2.504	2.555	2.607		
C_{sat} ($J\,K^{-1}mol^{-1}$)	241.0	245.9	250.9	256.0	261.3		

TABLE 11.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	85	68	2.730	1.35–1	0.55	1.35–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
85.0–385.3	537.40	–5.71710	1.77122	1.48250+1	4.61336		IV



Name: 2,4–Dimethylpentane
Formula: C_7H_{16}

CAS–RN: 108–08–7
Group No.: 11–018
Molar Mass: 100.20

TABLE 11.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30HUF/PAR2	160.2–294.4	15	1.00	not specified		C_p	BSIO	25PAR
61HUF/GRO	160.8–307.1	40	0.20	99.91	melpt	C_{sat}	BSAO	47HUF

TABLE 11.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61HUF/GRO	160.8–307.1	40	0.20#	0.175	8.52–3	0.03	6.68–6	–1
				Rejected data				
30HUF/PAR2	(1.54–1, 0.64, –1.35–1, –14)							

TABLE 11.18.3. Parameters of regression polynomial

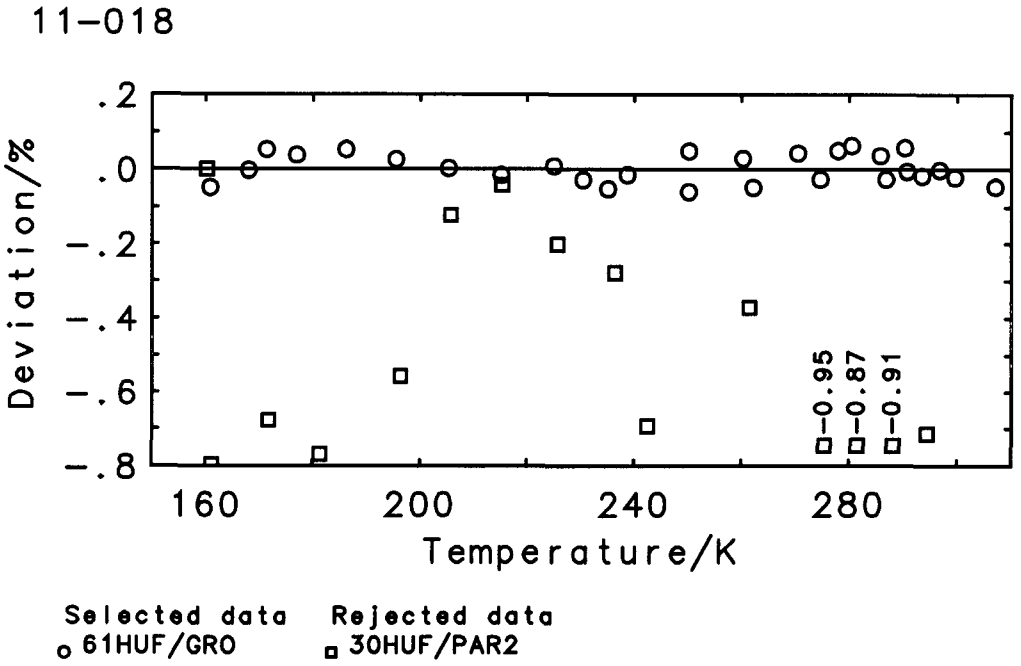
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	55	40	0.184	8.98–3	0.04	6.68–6	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
160.8–307.1	1.86799+1	–1.84428	2.13249	–1.94744–1			II

TABLE 11.18.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.692	1.722	1.754	1.787	1.822	1.859	1.898
C_{sat} (J K^{-1}mol^{-1})	169.5	172.5	175.7	179.1	182.6	186.3	190.2
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.937	1.979	2.021	2.064	2.109	2.123	2.154
C_{sat} (J K^{-1}mol^{-1})	194.1	198.3	202.5	206.8	211.3	212.7	215.8
Temp. (K)	290	298.15	300	310			
c_{sat} (J K^{-1}g^{-1})	2.200	2.238	2.247	2.295			
C_{sat} (J K^{-1}mol^{-1})	220.5	224.3	225.2	229.9			

TABLE 11.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	55	40	0.609	3.00–2	0.12	6.93–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
160.8–307.1	519.80	–6.75355	1.46590	1.33425+1	7.77858		II



Name: 3,3–Dimethylpentane
Formula: C_7H_{16}

CAS–RN: 562–49–2
Group No.: 11–019
Molar Mass: 100.20

TABLE 11.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
30HUF/PAR2	145.7–292.9	14	1.00	not specified	C_p	BSIO	25PAR
76FIN/MES	146.9–350.8	28	0.20	99.982 melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 11.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76FIN/MES	146.9–350.8	28	0.20	0.276	1.47–2	0.06	1.59–5	0
				Rejected data				
30HUF/PAR2	(1.19–1, 0.55, −1.07–1, −13)							

TABLE 11.19.3. Parameters of regression polynomial

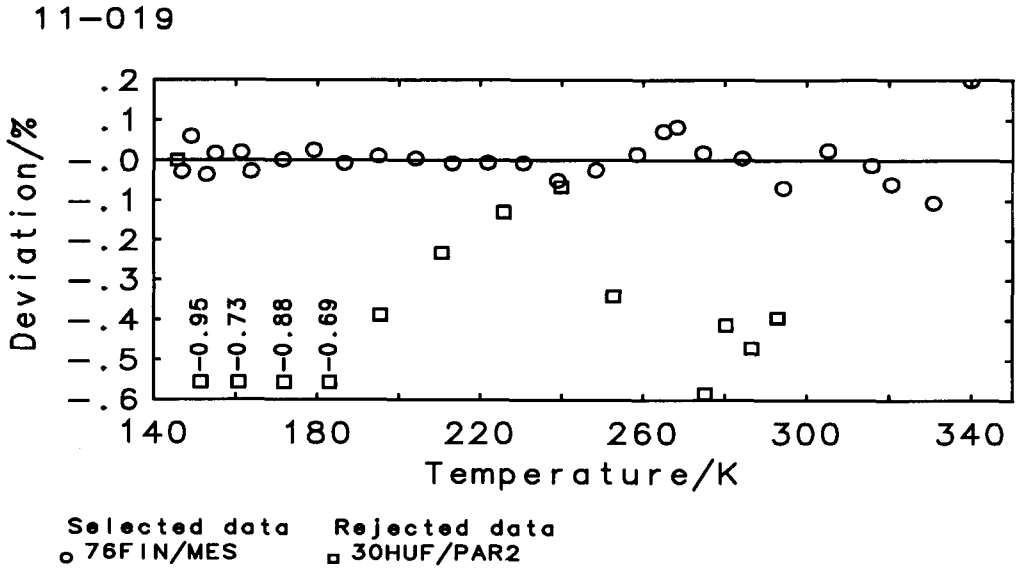
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	42	28	0.298	1.59–2	0.06	1.59–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
146.9–350.8		2.06869+1	-3.23326	2.10782	-1.48624-1		II

TABLE 11.19.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} ($J K^{-1} g^{-1}$)	1.666	1.684	1.705	1.728	1.754	1.781	1.810
C_{sat} ($J K^{-1} mol^{-1}$)	166.9	168.8	170.9	173.2	175.7	178.5	181.4
Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} ($J K^{-1} g^{-1}$)	1.841	1.875	1.910	1.946	1.985	2.024	2.037
C_{sat} ($J K^{-1} mol^{-1}$)	184.5	187.8	191.3	195.0	198.9	202.9	204.1
Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} ($J K^{-1} g^{-1}$)	2.066	2.109	2.145	2.153	2.198	2.245	2.293
C_{sat} ($J K^{-1} mol^{-1}$)	207.0	211.3	214.9	215.7	220.3	224.9	229.7
Temp. (K)	340	350					
c_{sat} ($J K^{-1} g^{-1}$)	2.341	2.391					
C_{sat} ($J K^{-1} mol^{-1}$)	234.6	239.6					

TABLE 11.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	42	28	1.883	8.97–2	0.38	5.61–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
146.9–350.8	536.40	-5.50206	2.66040	1.36968+1	2.84474		III



Name: 3–Ethylpentane
Formula: C_7H_{16}

CAS–RN: 617–78–7
Group No.: 11–020
Molar Mass: 100.20

TABLE 11.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
30HUF/PAR2	161.4–294.8	11	1.00	not specified	C_p	BSIO	25PAR
61HUF/GRO	161.2–298.8	44	nosp	99.995 melpt	C_{sat}	BSAO	47HUF
84FIL/LAU	293.0	1	2.00	98. anal	C_p	BDHO	84FIL/LAU

TABLE 11.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61HUF/GRO	161.2–298.8	44	0.20#	0.189	8.84–3	0.04	7.67–6	–1
				Rejected data				
30HUF/PAR2	(9.38–2, 0.38, –3.04–2, –3)			84FIL/LAU	(2.82, 9.73, 2.82, 1)			

TABLE 11.20.3. Parameters of regression polynomial

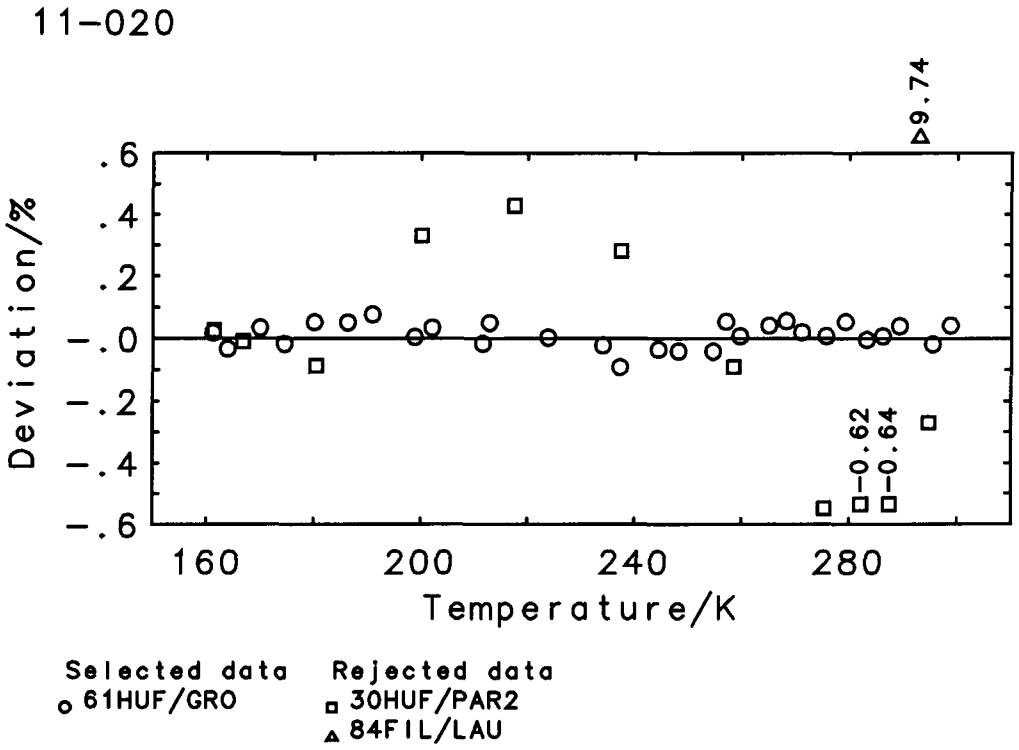
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	56	44	0.196	9.16–3	0.04	7.67–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
161.2–298.8		1.83550+1	3.45606–1	7.90238–1			II

TABLE 11.20.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.737	1.761	1.787	1.814	1.843	1.872	1.903
C_{sat} (J K^{-1}mol^{-1})	174.0	176.5	179.1	181.8	184.6	187.6	190.7
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.936	1.970	2.005	2.041	2.078	2.091	2.117
C_{sat} (J K^{-1}mol^{-1})	194.0	197.4	200.9	204.5	208.3	209.5	212.2
Temp. (K)	290	298.15	300				
c_{sat} (J K^{-1}g^{-1})	2.158	2.191	2.199				
C_{sat} (J K^{-1}mol^{-1})	216.2	219.6	220.4				

TABLE 11.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	56	44	0.300	1.44–2	0.06	1.56–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
161.2–298.8	540.60	–5.87119	2.44074	1.43331+1	3.53078		II



Name: Heptane
Formula: C_7H_{16}

CAS–RN: 142–82–5
Group No.: 11–021
Molar Mass: 100.20

TABLE 11.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24WIL/DAN		309.0–380.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
30PAR/HUF2		188.0–299.2	14	nosp	not specified		C_p	BSIO	25PAR
37VOL		298.1	1	nosp	not specified		C_p	BSIO	37VOL
39BYK		298.1–298.1	2	nosp	not specified		C_p	BSIT	39BYK
39PHI		300.8	1	nosp	not specified		C_p	BSIO	49WEI
40PIT2		194.6–317.6	6	0.50	99.85	melpt	C_p	BSIO	28LAT/GRE
47OSB/GIN	N	280.6–358.1	9S	0.10	99.96	estim	C_{sat}	BSAO	47OSB/GIN
47OSB/GIN		285.6–305.6	5S	0.10	99.96	estim	C_{sat}	BSAO	47OSB/GIN
54DOU/FUR	N	185.0–520.0	47S	0.10	99.999	melpt	C_{sat}	BSAO	45SCO/MEY
58SWI/ZIE1	N	332.6	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
61HUF/GRO	N	182.6–370.0	22S	0.20	not specified		C_{sat}	BSAO	47HUF
61MCC/MES	N	188.5–307.8	20	nosp	99.97	melpt	C_{sat}	BSAO	43RUE/HUF
61MCC/MES	N	183.0–320.8	25	nosp	99.996	melpt	C_{sat}	BSAO	43RUE/HUF
61MCC/MES	N	188.9–320.4	23	nosp	99.996	melpt	C_{sat}	BSAO	43RUE/HUF
61MCC/MES	N	192.9–340.8	17	nosp	99.996	melpt	C_{sat}	BSAO	43RUE/HUF
61MCC/MES	N	190.9–367.0	19	nosp	99.94	melpt	C_{sat}	BSAO	43RUE/HUF
66KLE		293.1–343.1	11S	0.10	not specified		C_p	BSAO	66KLE
70AKH		293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS
71AMI/ALI	N	373.1–538.2	21S	2.00	not specified		C_p	not specified	
72VAN		185.0–250.0	14S	0.50	99.968	melpt	C_p	BSAO	72VAN
75GRI/RAS	N	303.5–342.8	3	nosp	not specified		C_p	BDAO	75RAS/GRI
75HOL/ZIE		182.0–312.0	eqn	0.20	99.73	anal	C_p	BSAO	45SCO/MEY
75SAN	N	413.1–513.2	8S	1.00	not specified		C_p	FSIO	75SAN
77MEI/BLO		187.0–354.6	35	nosp	not specified		C_{sat}	BSAO	72VAN
79BRO/ZIE		183.0–302.0	eqn	nosp	99.7	melpt	C_p	BSAO	45SCO/MEY
79SCH/OFF		190.0–285.0	20S	nosp	99.88	melpt	C_{sat}	BSAO	79SCH/OFF
80KAL/JED		185.0–301.0	96	0.20	99.95	chrom	C_p	BSAO	80KAL/JED
83TAN/ZHO		214.2–365.2	40	0.20	99.99	chrom	C_{sat}	BSAO	83TAN/ZHO
84GRI/AND		293.0–323.6	14	0.50	not specified		C_p	BSAO	67RAS/GAN
84GUS/MIR		303.1–363.1	4S	1.60	not specified		C_p	BDHT	84GUS/MIR
85CZA		299.3	1	nosp	not specified		C_p	BSIO	79CZA
87VAN/VAN		184.2–345.7	37	0.20	99.75	melpt	C_p	BSAO	87VAN/VAN
87WIL/ING		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
88MEL/VER		193.1–523.2	11	2.50	not specified		C_{sat}	not specified	

47OSB/GIN calorimeter with a vessel of large volume
54DOU/FUR same data in 53GIN/FUR
58SWI/ZIE1 average value in temperature range 294–369 K
61HUF/GRO same data in 67MES/GUT
61MCC/MES measured in 1947
61MCC/MES measured in 1949
61MCC/MES measured in 1951(A)
61MCC/MES measured in 1951(B); results less accurate near and above room temperature
61MCC/MES measured in 1954
71AMI/ALI calculated from Cv measured at the saturation line
75GRI/RAS grade: pure
75SAN same data in 76SAN/MEL; C_p at the saturation pressure extrapolated from high pressure measurement

TABLE 11.21.2a. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54DOU/FUR	185.0–370.0	32	0.10	0.092	2.35–3	0.01	–1.78–3	–9
54DOU/FUR	380.0–480.0	11	0.30	0.053	5.78–3	0.02	1.44–3	3
61HUF/GRO	182.6–370.0	22	0.20	0.304	1.58–2	0.06	1.00–2	14

TABLE 11.21.2b. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54DOU/FUR	200.0–520.0	44	0.10	7.832	2.57–1	0.78	–1.68–2	–4
61HUF/GRO	200.0–370.0	20	0.10	6.914	1.76–1	0.69	–1.46–2	–4
				Rejected data				
24WIL/DAN	(6.03–1, 2.19, –2.07–1, –1)			30PAR/HUF2	(3.71–1, 1.44, –2.67–1, –9)			
37VOL	(3.72–1, 1.39, –3.72–1, –1)			39BYK	(1.69, 6.65, –1.69, –2)			
39PHI	(1.90, 7.49, –1.90, –1)			40PIT2	(6.55–2, 0.26, 4.29–3, 1)			
47OSB/GIN	(1.09–1, 0.40, –2.61–2, –1)			47OSB/GIN	(1.39–1, 0.52, –1.37–1, –5)			
58SWI/ZIE1	(1.10, 3.68, 1.10, 1)			61MCC/MES	(1.88–1, 0.74, –8.78–2, –10)			
61MCC/MES	(2.04–1, 0.83, 3.54–2, 1)			61MCC/MES	(1.76–1, 0.71, –2.64–2, –8)			
61MCC/MES	(1.87–1, 0.74, –5.73–2, –10)			61MCC/MES	(1.06, 3.62, 2.62–1, –2)			
66KLE	(9.09–2, 0.33, –4.96–2, –4)			70AKH	(2.29–1, 0.86, –2.29–1, –1)			
71AMI/ALI	(7.68–1, 2.12, –5.76–1, –11)			72VAN	(2.56–1, 1.05, 7.64–2, 1)			
75GRI/RAS	(1.84–1, 0.66, –1.73–2, 1)			75HOL/ZIE	(1.72–1, 0.67, –1.18–1, –2)			
75SAN	(9.64–1, 2.57, –7.24–1, –6)			77MEI/BLO	(1.53–1, 0.62, –4.93–2, –15)			
79BRO/ZIE	(1.00, 3.95, –9.95–1, –2)			79SCH/OFF	(2.08–1, 0.83, –6.74–2, –8)			
80KAL/JED	(1.94–1, 0.77, –8.04–2, –40)			83TAN/ZHO	(1.88–1, 0.73, –1.35–1, –24)			
84GRI/AND	(3.18–1, 1.14, 3.10–1, 14)			84GUS/MIR	(3.76–1, 1.33, –3.64–1, –4)			
85CZA	(8.58–2, 0.32, –8.58–2, –1)			87VAN/VAN	(1.67–1, 0.65, –1.02–1, –18)			
87WIL/ING	(1.31–1, 0.48, –1.31–1, –1)			88MEL/VER	(2.09–1, 0.70, 4.56–2, –1)			

TABLE 11.21.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	65	0.199	1.01–2	0.04	2.77–3	8
C_{sat}	65	65	0.197	9.80–3	0.04	2.71–3	2

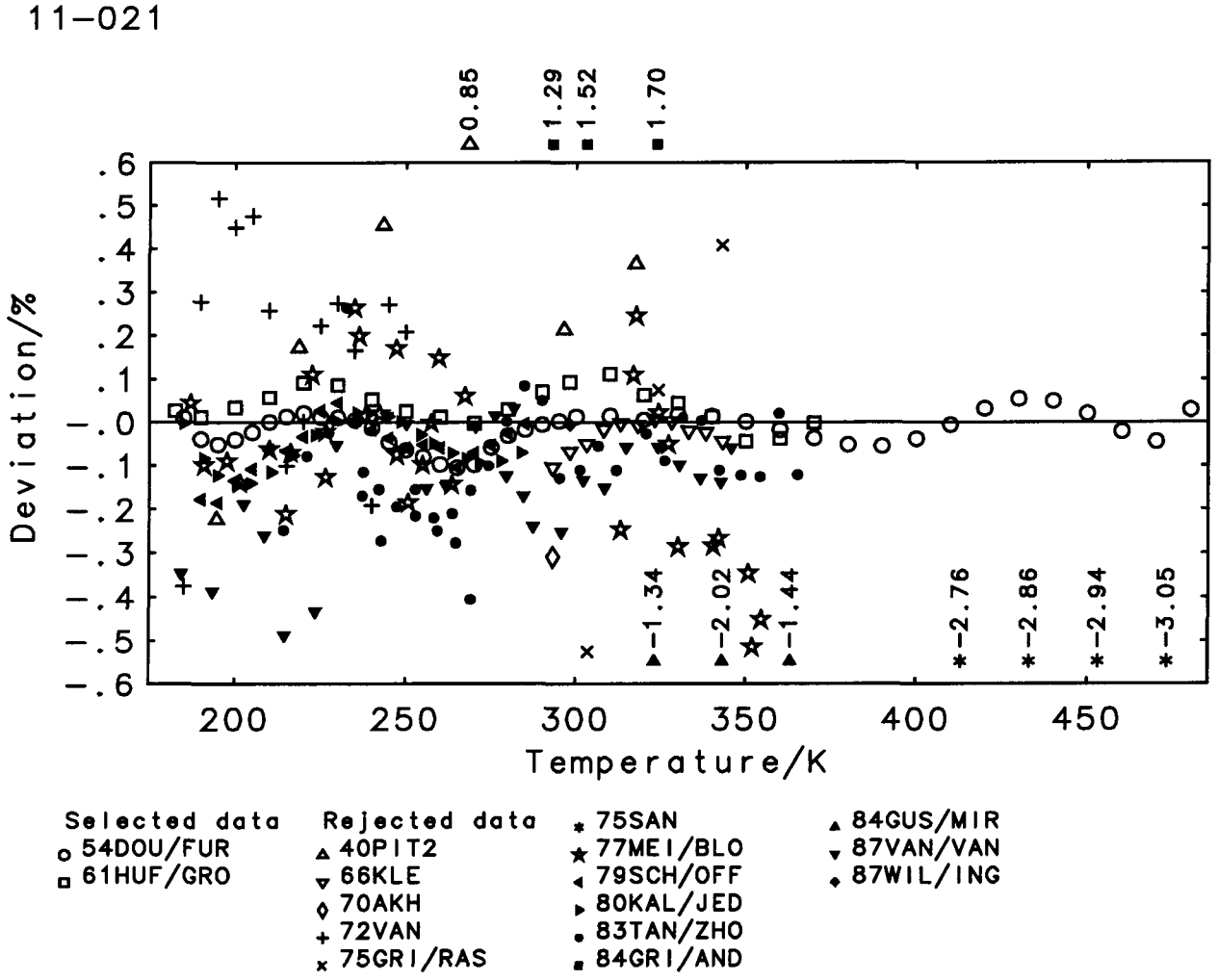
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
182.6–260.0	6.11411+1	–4.53403+1	1.76764+1	–2.11880	I
260.0–400.0	2.54134+1	–4.11613	1.82098	–8.60461–2	I
400.0–480.0	–8.76637+1	8.06917+1	–1.93810+1	1.68078	I
182.6–260.0	6.09258+1	–4.50536+1	1.75504+1	–2.10051	I
260.0–400.0	2.62792+1	–5.07669	2.17466	–1.29263–1	I
400.0–480.0	–4.11778+1	4.55161+1	–1.04735+1	9.24753–1	I

TABLE 11.21.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	2.0142	2.0094	2.0128	2.0235	2.0402	2.0620	2.0878
C_p ($J\,K^{-1}mol^{-1}$)	201.82	201.34	201.69	202.75	204.43	206.62	209.20
c_{sat} ($J\,K^{-1}g^{-1}$)	2.0142	2.0094	2.0128	2.0235	2.0402	2.0620	2.0878
C_{sat} ($J\,K^{-1}mol^{-1}$)	201.82	201.35	201.68	202.75	204.43	206.62	209.20
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.1167	2.1476	2.1577	2.1803	2.2149	2.2444	2.2512
C_p ($J\,K^{-1}mol^{-1}$)	212.09	215.19	216.21	218.47	221.93	224.89	225.58
c_{sat} ($J\,K^{-1}g^{-1}$)	2.1167	2.1476	2.1577	2.1803	2.2149	2.2444	2.2513
C_{sat} ($J\,K^{-1}mol^{-1}$)	212.09	215.19	216.21	218.47	221.93	224.89	225.59
Temp. (K)	310	320	330	340	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	2.2892	2.3291	2.3706	2.4136	2.4582	2.5043	2.5519
C_p ($J\,K^{-1}mol^{-1}$)	229.39	233.38	237.53	241.85	246.32	250.94	255.71
c_{sat} ($J\,K^{-1}g^{-1}$)	2.2892	2.3289	2.3701	2.4128	2.4568	2.5023	2.5490
C_{sat} ($J\,K^{-1}mol^{-1}$)	229.38	233.36	237.49	241.76	246.18	250.73	255.41
Temp. (K)	380	390	400	410	420	430	440
c_p ($J\,K^{-1}g^{-1}$)	2.6010	2.6514	2.7032	2.756	2.812	2.870	2.932
C_p ($J\,K^{-1}mol^{-1}$)	260.62	265.68	270.87	276.2	281.8	287.6	293.8
c_{sat} ($J\,K^{-1}g^{-1}$)	2.5969	2.6461	2.6963	2.748	2.800	2.855	2.912
C_{sat} ($J\,K^{-1}mol^{-1}$)	260.22	265.14	270.17	275.3	280.6	286.1	291.8
Temp. (K)	450	460	470	480			
c_p ($J\,K^{-1}g^{-1}$)	2.999	3.072	3.151	3.237			
C_p ($J\,K^{-1}mol^{-1}$)	300.5	307.8	315.7	324.3			
c_{sat} ($J\,K^{-1}g^{-1}$)	2.973	3.036	3.103	3.175			
C_{sat} ($J\,K^{-1}mol^{-1}$)	297.9	304.2	310.9	318.1			

TABLE 11.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	542	64	7.805	2.43–1	0.78	–1.61–2	–8
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
200.0–520.0	540.15	–4.08402	1.74311–1	1.93025+1	3.65193	5.97785	2.07661	IV



Name: 2–Methylhexane
Formula: C_7H_{16}

CAS–RN: 591–76–4
Group No.: 11–022
Molar Mass: 100.20

TABLE 11.22.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF2		160.0–292.4	12	1.00	not specified		C_p	BSIO	25PAR
61HUF/GRO	N	160.4–301.2	19	0.20	99.84	melpt	C_{sat}	BSAO	47HUF
84FIL/LAU		293.0	1	2.00	99.	anal	C_p	BDHO	84FIL/LAU

61HUF/GRO smoothed values in 71MES/FIN

TABLE 11.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61HUF/GRO	160.4–301.2	19	0.20	0.159	8.11–3	0.03	2.91–6	1
				Rejected data				
30PAR/HUF2	(9.54–2, 0.39, –1.02–2, –1)			84FIL/LAU	(5.52–1, 2.13, –5.52–1, –1)			

TABLE 11.22.3. Parameters of regression polynomial

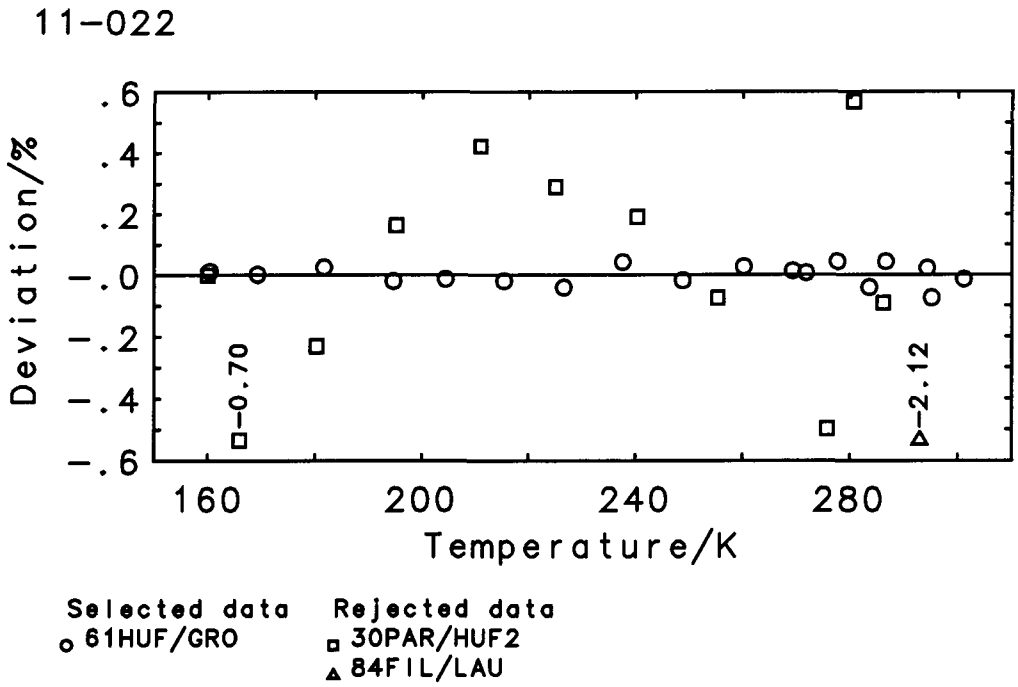
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	32	19	0.174	8.84–3	0.03	2.91–6	1
Temp. range K	A_1	A_2	A_3				Level of uncertainty
160.4–301.2	2.09916+1	–1.30228	1.09026				II

TABLE 11.22.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} ($J K^{-1} g^{-1}$)	1.800	1.820	1.840	1.863	1.888	1.914	1.942
C_{sat} ($J K^{-1} mol^{-1}$)	180.4	182.3	184.4	186.7	189.1	191.8	194.6
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} ($J K^{-1} g^{-1}$)	1.972	2.004	2.037	2.072	2.110	2.122	2.148
C_{sat} ($J K^{-1} mol^{-1}$)	197.6	200.8	204.1	207.7	211.4	212.6	215.3
Temp. (K)	290	298.15	300				
c_{sat} ($J K^{-1} g^{-1}$)	2.189	2.224	2.232				
C_{sat} ($J K^{-1} mol^{-1}$)	219.4	222.8	223.6				

TABLE 11.22.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	32	19	0.580	2.83–2	0.12	4.93–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
160.4–301.2	530.40	–2.87205	4.35021	1.42552+1	4.74040–1		II



Name: 3–Methylhexane
Formula: C_7H_{16}

CAS–RN: 589–34–4
Group No.: 11–023
Molar Mass: 100.20

TABLE 11.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30HUF/PAR2	99.1–289.2	11	1.00	not specified		C_p	BSIO	25PAR
36PAR/THO	91.0–289.2	26	1.00	not specified		C_p	BSIO	25PAR

TABLE 11.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
30HUF/PAR2	99.1–289.2	11	1.00	0.347	8.61–2	0.35	–3.16–2	–3
36PAR/THO	91.0–289.2	26	1.00	0.222	5.22–2	0.22	1.38–2	5

TABLE 11.23.3. Parameters of regression polynomial

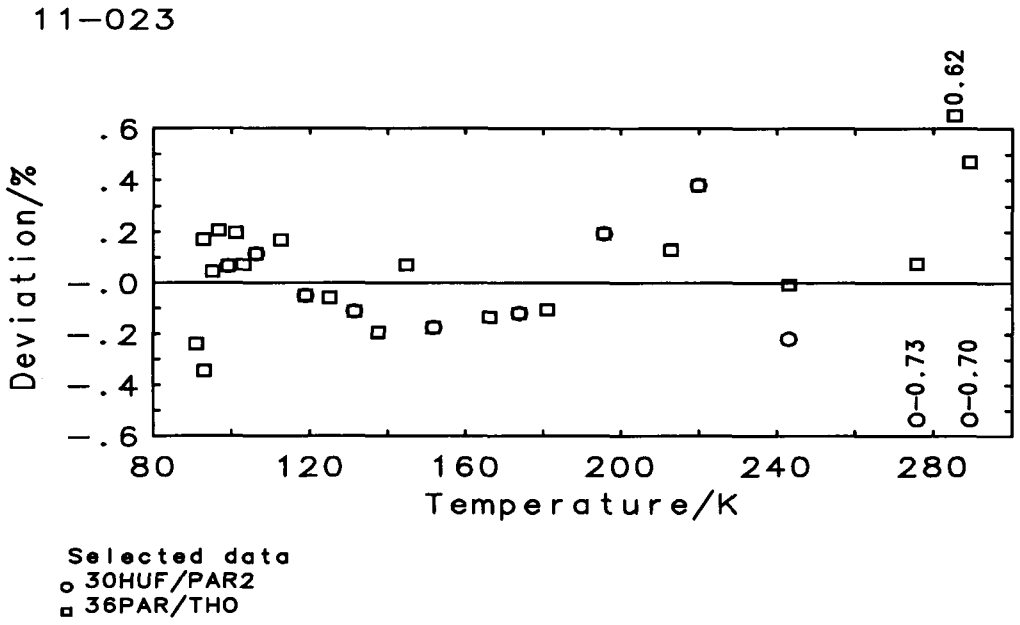
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	37	0.277	6.69–2	0.28	3.19–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
91.0–289.2		1.98577+1	–7.93355–1	1.00239			IV

TABLE 11.23.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_p (J K^{-1}g^{-1})	1.656	1.665	1.676	1.688	1.703	1.719	1.736
C_p (J K^{-1}mol^{-1})	165.9	166.8	167.9	169.2	170.6	172.2	174.0
Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.755	1.776	1.799	1.823	1.849	1.876	1.905
C_p (J K^{-1}mol^{-1})	175.9	178.0	180.2	182.7	185.3	188.0	190.9
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.936	1.969	2.003	2.039	2.076	2.088	2.115
C_p (J K^{-1}mol^{-1})	194.0	197.3	200.7	204.3	208.1	209.3	212.0
Temp. (K)	290	298.15					
c_p (J K^{-1}g^{-1})	2.156	2.191					
C_p (J K^{-1}mol^{-1})	216.1	219.5					

TABLE 11.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	37	0.391	8.96–2	0.39	2.22–3	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
91.0–289.2	535.30	2.83394	7.94241	1.08092+1	2.52795–1		IV



Name: 2,2,3–Trimethylbutane
Formula: C_7H_{16}

CAS–RN: 464–06–2
Group No.: 11–024
Molar Mass: 100.20

TABLE 11.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30HUF/PAR2	253.2–293.9	6	1.00	not specified		C_p	BSIO	25PAR
61HUF/GRO	253.0–313.3	10	0.20	99.95	melpt	C_{sat}	BSAO	47HUF

TABLE 11.24.2. Correlated heat capacities

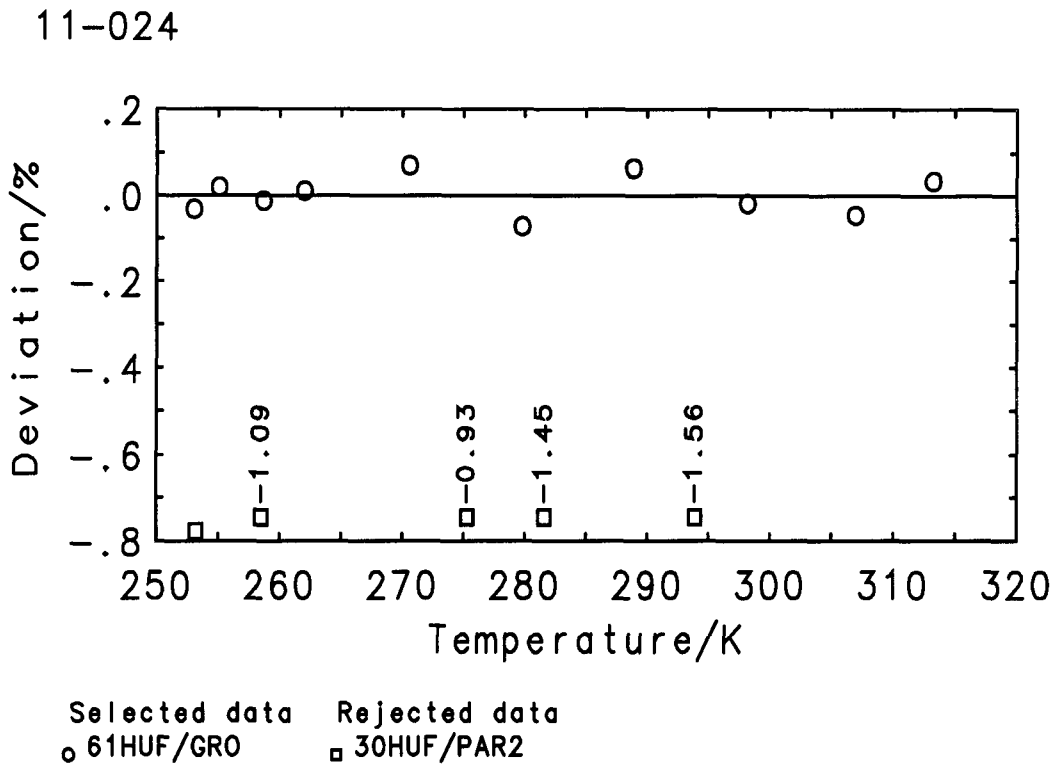
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61HUF/GRO	253.0–313.3	10	0.20	0.220	1.10–2	0.04	8.39–6	–1
				Rejected data				
30HUF/PAR2	(3.03–1, 1.25, –2.93–1, –6)							

TABLE 11.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	10	0.246	1.22–2	0.05	8.39–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
253.0–313.3		1.00856+1	5.22893				II

TABLE 11.24.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.922	1.965	2.008	2.022	2.052	2.095	2.130
C_{sat} (J K^{-1}mol^{-1})	192.5	196.9	201.2	202.6	205.6	209.9	213.5
Temp. (K)	300	310					
c_{sat} (J K^{-1}g^{-1})	2.138	2.182					
C_{sat} (J K^{-1}mol^{-1})	214.3	218.6					



Name: 2,3-Dimethylhexane
Formula: C_8H_{18}

CAS-RN: 584-94-1
Group No.: 11-025
Molar Mass: 114.23

TABLE 11.25.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84FIL/LAU	293.00	2.190	2.00	99.0	estim	C_p	BDHO	84FIL/LAU

Name: 2,5-Dimethylhexane
Formula: C_8H_{18}

CAS-RN: 592-13-2
Group No.: 11-026
Molar Mass: 114.23

TABLE 11.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47OSB/GIN	285.6-313.1	4S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN
84FIL/LAU	293.0	1	2.00	95.0	estim	C_p	BDHO	84FIL/LAU

TABLE 11.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47OSB/GIN	285.6–313.1	4	0.30#	0.964	8.74–2	0.29	4.72–4	0
				Rejected data				
84FIL/LAU	(6.58–1, 2.17, 6.58–1, 1)							

TABLE 11.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	4	1.363	1.24–1	0.41	4.72–4	0
Temp. range K		A_1	A_2				Level of uncertainty
285.6–313.1		1.02999+1	6.59931				III

TABLE 11.26.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310
c_{sat} ($J K^{-1} g^{-1}$)	2.095	2.143	2.182	2.191	2.239
C_{sat} ($J K^{-1} mol^{-1}$)	239.3	244.8	249.2	250.2	255.7

Name: 3,3–Dimethylhexane
Formula: C_8H_{18}

CAS–RN: 563–16–6
Group No.: 11–027
Molar Mass: 114.23

TABLE 11.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47OSB/GIN	290.6–305.6	4S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN

TABLE 11.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	0.660	1.98–2	0.07	1.76–5	I
Temp. range K		A_1	A_2				Level of uncertainty
290.6–305.6		–8.57274	1.28264+1				II

TABLE 11.27.4. Recommended values of heat capacities

Temp. (K)	290	295	298.15	300	305
c_{sat} ($J K^{-1} g^{-1}$)	2.083	2.130	2.160	2.177	2.223
C_{sat} ($J K^{-1} mol^{-1}$)	238.0	243.3	246.7	248.7	254.0

Name: 3–Ethyl–2–methylpentane
Formula: C_8H_{18}

CAS–RN: 609–26–7
Group No.: 11–028
Molar Mass: 114.23

TABLE 11.28.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84FIL/LAU	293.00	2.248	2.00	99.0	estim	C_p	BDHO	84FIL/LAU

Name: 2–Methylheptane
Formula: C_8H_{18}

CAS–RN: 592–27–8
Group No.: 11–029
Molar Mass: 114.23

TABLE 11.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47OSB/GIN	285.6–305.6	5S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN
71MES/FIN	177.6–369.6	23	0.20	99.969	melpt	C_{sat}	BSAO	43RUE/HUF
84FIL/LAU	293.0	1	2.00	99.	anal	C_p	BDHO	84FIL/LAU

TABLE 11.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47OSB/GIN	285.6–305.6	5	0.10	0.609	1.86–2	0.06	–1.32–2	–3
71MES/FIN	177.6–369.6	23	0.20#	0.486	2.76–2	0.10	1.15–2	11
				Rejected data				
84FIL/LAU	(1.32–1, 0.44, 1.32–1, 1)							

TABLE 11.29.3. Parameters of regression polynomial

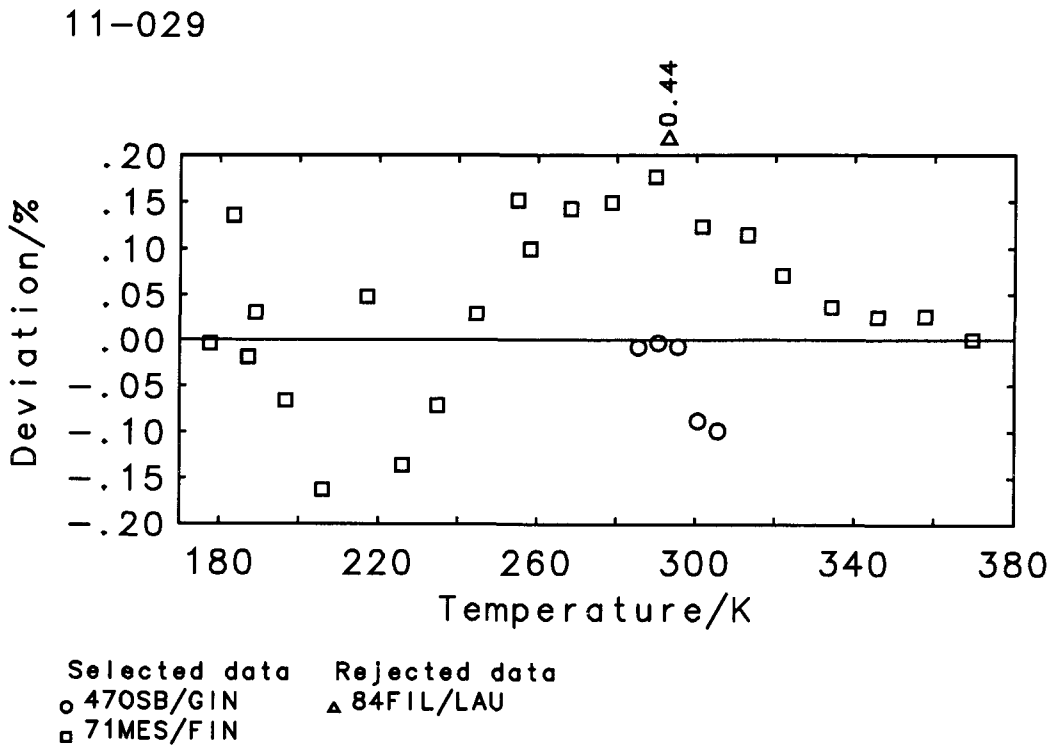
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	29	28	0.550	2.83–2	0.10	7.11–3	8
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
177.6–369.6	3.06623+1	–8.37686	3.62516	–2.88494–1			II

TABLE 11.29.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} ($J\,K^{-1}g^{-1}$)	1.867	1.882	1.900	1.921	1.944	1.970	1.998
C_{sat} ($J\,K^{-1}mol^{-1}$)	213.2	215.0	217.0	219.4	222.1	225.0	228.2
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J\,K^{-1}g^{-1}$)	2.029	2.061	2.096	2.107	2.132	2.171	2.203
C_{sat} ($J\,K^{-1}mol^{-1}$)	231.7	235.4	239.4	240.7	243.6	247.9	251.6
Temp. (K)	300	310	320	330	340	350	360
c_{sat} ($J\,K^{-1}g^{-1}$)	2.210	2.252	2.295	2.339	2.384	2.430	2.477
C_{sat} ($J\,K^{-1}mol^{-1}$)	252.5	257.2	262.1	267.1	272.3	277.6	282.9
Temp. (K)	370						
c_{sat} ($J\,K^{-1}g^{-1}$)	2.524						
C_{sat} ($J\,K^{-1}mol^{-1}$)	288.4						

TABLE 11.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	29	28	2.238	1.24–1	0.42	–1.10–2	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
177.6–369.6	559.60	–4.68388	3.83163	1.76597+1	1.43142		III



Name: 3-Methylheptane
Formula: C_8H_{18}

CAS-RN: 589-81-1
Group No.: 11-030
Molar Mass: 114.23

TABLE 11.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47OSB/GIN	285.6–305.6	5S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN
73FIN/MES	157.2–376.0	28	0.20	99.973	melpt	C_{sat}	BSAO	43RUE/HUF
84FIL/LAU	293.0	1	2.00	97.	anal	C_p	BDHO	84FIL/LAU

TABLE 11.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47OSB/GIN	285.605.6	5	0.20#	0.745	4.45–2	0.15	–4.42–2	–5
73FIN/MES	157.2–376.0	28	0.20#	0.438	2.62–2	0.09	7.97–3	5
				Rejected data				
84FIL/LAU	(1.73–1, 0.58, 1.73–1, 1)							

TABLE 11.30.3. Parameters of regression polynomial

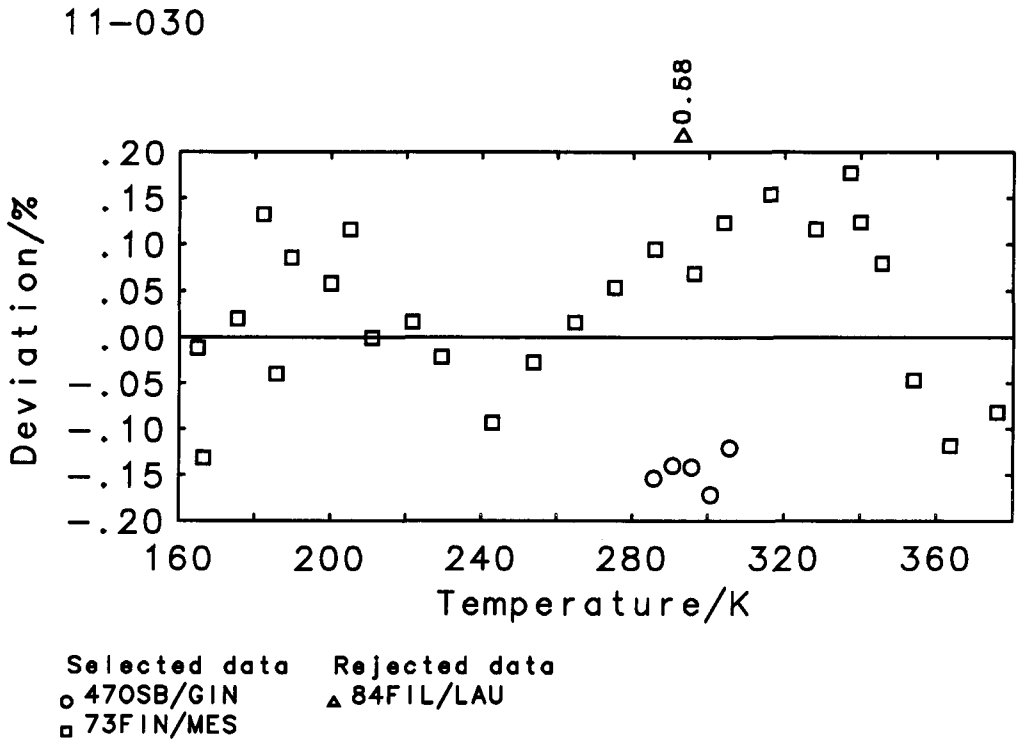
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	33	0.530	3.17–2	0.11	5.97–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
157.2–376.0		2.55387+1	–3.63138	2.14998	–1.41712–1		II

TABLE 11.30.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J $K^{-1}g^{-1}$)	1.794	1.811	1.830	1.851	1.874	1.898	1.925
C_{sat} (J $K^{-1}mol^{-1}$)	205.0	206.9	209.0	211.4	214.0	216.9	219.9
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J $K^{-1}g^{-1}$)	1.953	1.983	2.015	2.048	2.083	2.094	2.119
C_{sat} (J $K^{-1}mol^{-1}$)	223.1	226.6	230.2	234.0	237.9	239.2	242.1
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J $K^{-1}g^{-1}$)	2.157	2.189	2.196	2.236	2.278	2.320	2.364
C_{sat} (J $K^{-1}mol^{-1}$)	246.4	250.0	250.8	255.4	260.2	265.0	270.0
Temp. (K)	350	360	370	380			
c_{sat} (J $K^{-1}g^{-1}$)	2.409	2.454	2.501	2.548			
C_{sat} (J $K^{-1}mol^{-1}$)	275.1	280.3	285.7	291.1			

TABLE 11.30.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	33	1.867	1.08–1	0.37	7.45–3	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
157.2–376.0	563.70	–6.47015	2.46348	1.76550+1	4.24835		III



Name: 4–Methylheptane
Formula: C_8H_{18}

CAS–RN: 589–53–7
Group No.: 11–031
Molar Mass: 114.23

TABLE 11.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47OSB/GIN	285.6–313.1	4S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN

TABLE 11.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	1.339	1.22–1	0.40	4.56–4	0
Temp. range K		A_1	A_2				Level of uncertainty
285.6–313.1		1.05644+1	6.58446				III

TABLE 11.31.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.111	2.159	2.198	2.207	2.255
C_{sat} (J K^{-1}mol^{-1})	241.1	246.6	251.1	252.1	257.6

Name: Octane
Formula: C_8H_{18}

CAS-RN: 111-65-9
Group No.: 11-032
Molar Mass: 114.23

TABLE 11.32.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*98LOU	N	344.9	1	nosp	not specified		avg	DSIO	*98LOU
30PAR/HUF2		223.0–293.7	8	nosp	not specified		C_p	BSIO	25PAR
31HUF/PAR		227.0–298.3	5	nosp	not specified		C_p	BSIO	25PAR
47OSB/GIN		285.6–305.6	5S	0.10	99.96	estim	C_{sat}	BSAO	47OSB/GIN
49TSC/WET		298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
51CON/SAG		299.8–366.5	13S	nosp	not specified		C_p	BSAO	39SAG/EVA
54FIN/GRO2	N	222.6–297.6	18	0.20	99.94	melpt	C_{sat}	BSAO	43RUE/HUF
61ROU		283.1–312.3	15	nosp	99.83	anal	C_p	BSAO	61ROU
70AKH		293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS
71AMI/ALI	N	403.1–567.2	21S	2.00	not specified		C_p	not specified	
75GRI/RAS	N	303.9–462.1	9	1.00	not specified		C_p	BDAO	75RAS/GRI
77NAZ/MUS		303.2–383.2	5	1.50	not specified		C_p	BSAO	77NAZ/MUS
80SHA/LYU		216.4–300.0	12S	0.50	99.57	melpt	C_p	BSAO	80SHA/LYU
81GRO/ING		298.1	1	nosp	99.0	chrom	C_p	FSIT	71PIC/LED
84GRI/AND	N	297.5–386.1	7	0.50	not specified		C_p	BSAO	67RAS/GAN
84ROU/GRO		298.1	1	0.30	99.	estim	C_p	FSIT	71PIC/LED
85COS/PAT2		298.2	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
85LAI/GRO		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
85LAI/ROD		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
86BEN/DAR1		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	98.8	chrom	C_p	BDCT	91BAN/GAR
91OGA/MIT		298.1	1	nosp	not specified		C_p	FSIO	85OGA
91SOE/NAK		298.1	1	nosp	99.99	chrom	C_p	FSIO	85OGA
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED

*98LOU average value in temperature range 294–396 K
54FIN/GRO2 smoothed data in 67MES/GUT
71AMI/ALI calculated from C_v measured at the saturation line
75GRI/RAS grade: pure; the last five values at pressures higher than vapour pressure
84GRI/AND grade: pure

TABLE 11.32.2. *Correlated heat capacities*

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47OSB/GIN	285.6–305.6	5	0.30#	1.444	1.33–1	0.43	1.32–1	5
49TSC/WET	298.1	1	0.50#	0.820	1.26–1	0.41	1.26–1	1
54FIN/GRO2	222.6–297.6	18	0.20	0.706	4.26–2	0.14	–1.90–2	–3
75GRI/RAS	304.0–462.1	9	1.00	0.510	1.73–1	0.51	–6.58–2	–3
77NAZ/MUS	303.2–383.2	5	1.50	0.080	3.94–2	0.12	–2.42–2	–1
85COS/PAT2	298.2	1	0.50#	0.415	6.39–2	0.21	6.39–2	1
85LAI/GRO	298.1	1	0.50#	0.257	3.93–2	0.13	–3.93–2	–1
86BEN/DAR1	298.1	1	0.50#	0.013	2.06–3	0.01	–2.06–3	0
91OGA/MIT	298.1	1	0.30#	1.098	1.01–1	0.33	1.01–1	1
91TRE/COS	298.1	1	0.50#	0.433	6.65–2	0.22	6.65–2	1
				Rejected data				
*98LOU	(1.40–3, 0.00, –1.40–3, 0)				30PAR/HUF2	(4.84–1, 1.67, –4.68–1, –8)		
31HUF/PAR	(3.74–1, 1.28, –3.69–1, –5)				51CON/SAG	(5.69–1, 1.75, –5.45–1, –13)		
61ROU	(3.43–1, 1.14, –2.18–1, –9)				70AKH	(2.13–1, 0.69, 2.13–1, 1)		
71AMI/ALI	(1.36, 3.63, –1.33, –6)				80SHA/LYU	(1.45–1, 0.48, –5.94–2, 0)		
81GRO/ING	(1.27–1, 0.42, –1.27–1, –1)				84GRI/AND	(3.29–1, 0.99, –3.22–1, –7)		
84ROU/GRO	(1.33–1, 0.44, –1.33–1, –1)				85LAI/ROD	(1.69–1, 0.55, –1.69–1, –1)		
91BAN/GAR	(1.61–1, 0.49, –1.47–1, –12)				91SOE/NAK	(1.12–1, 0.36, –1.12–1, –1)		
92LAI/ROD	(1.89–1, 0.62, –1.89–1, –1)							

TABLE 11.32.3. *Parameters of cubic spline polynomials*

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	143	43	0.796	1.07–1	0.33	–1.79–3	1
C_{sat}	143	43	0.795	1.07–1	0.33	–2.03–3	1

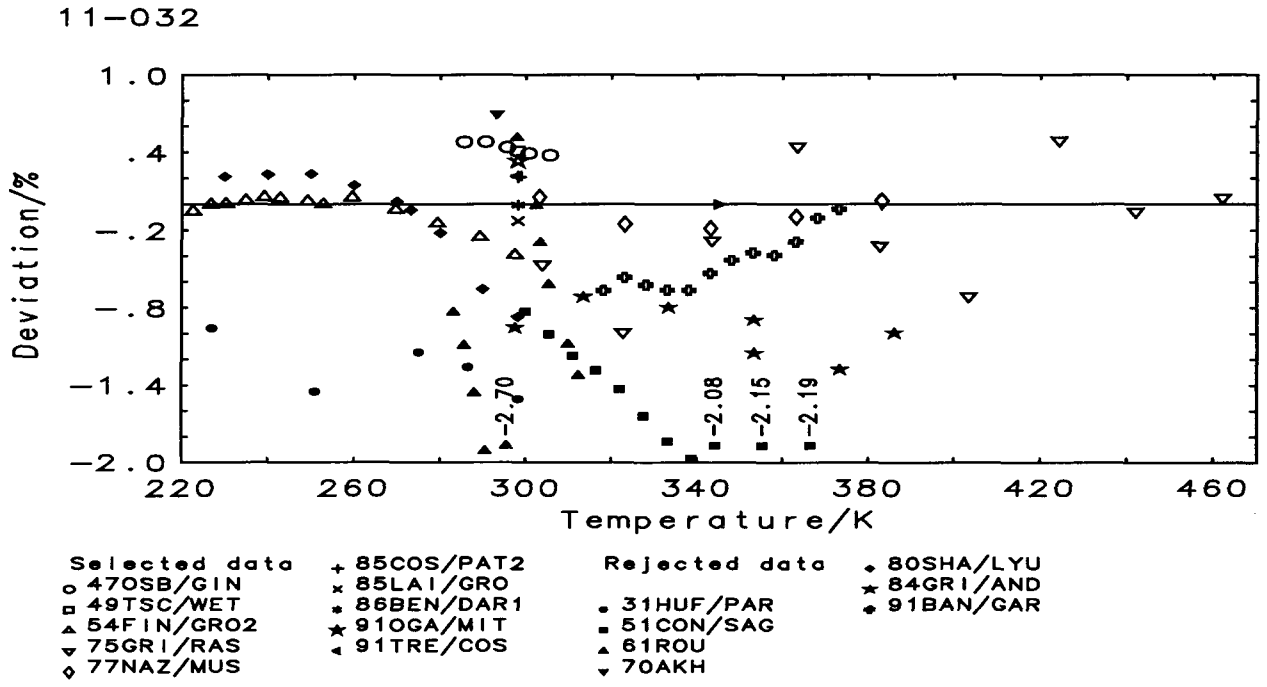
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
222.6–300.0	7.59487+1	–5.42060+1	1.93384+1	–2.09614	II
300.0–462.1	1.52779+1	6.46485	–8.85159–1	1.50930–1	IV
222.6–300.0	7.57257+1	–5.39481+1	1.92395+1	–2.08356	II
300.0–462.1	1.70184+1	4.75936	–3.29600–1	9.07863–2	IV

TABLE 11.32.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J\,K^{-1}g^{-1}$)	2.036	2.043	2.057	2.078	2.103	2.134	2.144
C_p ($J\,K^{-1}mol^{-1}$)	232.6	233.4	235.0	237.4	240.3	243.7	244.9
c_{sat} ($J\,K^{-1}g^{-1}$)	2.036	2.043	2.057	2.078	2.103	2.133	2.144
C_{sat} ($J\,K^{-1}mol^{-1}$)	232.6	233.4	235.0	237.4	240.3	243.7	244.9
Temp. (K)	**280**	**290**	**298.15**	**300**	**310**	**320**	**330**
c_p ($J\,K^{-1}g^{-1}$)	2.167	2.203	2.233	2.240	2.279	2.318	2.358
C_p ($J\,K^{-1}mol^{-1}$)	247.5	251.6	255.1	255.9	260.3	264.8	269.4
c_{sat} ($J\,K^{-1}g^{-1}$)	2.167	2.203	2.233	2.240	2.279	2.318	2.358
C_{sat} ($J\,K^{-1}mol^{-1}$)	247.5	251.6	255.1	255.9	260.3	264.8	269.4
Temp. (K)	**340**	**350**	**360**	**370**	**380**	**390**	**400**
c_p ($J\,K^{-1}g^{-1}$)	2.399	2.441	2.484	2.528	2.573	2.619	2.666
C_p ($J\,K^{-1}mol^{-1}$)	274.0	278.8	283.7	288.7	293.9	299.2	304.6
c_{sat} ($J\,K^{-1}g^{-1}$)	2.399	2.441	2.483	2.527	2.571	2.617	2.663
C_{sat} ($J\,K^{-1}mol^{-1}$)	274.0	278.8	283.7	288.6	293.7	298.9	304.2
Temp. (K)	**410**	**420**	**430**	**440**	**450**	**460**	
c_p ($J\,K^{-1}g^{-1}$)	2.715	2.766	2.818	2.871	2.926	2.983	
C_p ($J\,K^{-1}mol^{-1}$)	310.2	315.9	321.9	328.0	334.2	340.7	
c_{sat} ($J\,K^{-1}g^{-1}$)	2.711	2.760	2.810	2.861	2.914	2.968	
C_{sat} ($J\,K^{-1}mol^{-1}$)	309.7	315.3	321.0	326.9	332.9	339.0	

TABLE 11.32.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	143	43	2.106	2.31–1	0.70	9.14–2	14
Temp. range K	**T_c K**	**A_1**	**A_2**	**A_3**	**A_4**		**Level of uncertainty**
222.6–462.1	568.95	–5.81193	9.16902–1	1.95769+1	9.20996		IV



Name: 2,2,3,3–Tetramethylbutane
Formula: C_8H_{18}

CAS–RN: 594–82–1
Group No.: 11–033
Molar Mass: 114.23

TABLE 11.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52SCO/DOU	375.4–378.0	3	0.20	99.976	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 11.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	3	3	0.353	2.39–2	0.07	1.14–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
375.4–378.0		5.74080	7.44551				II

TABLE 11.33.4. Recommended values of heat capacities

Temp. (K)	375	378
c_{sat} (J $K^{-1}g^{-1}$)	2.450	2.466
C_{sat} (J $K^{-1}mol^{-1}$)	279.9	281.7

Name: 2,2,4–Trimethylpentane
Formula: C_8H_{18}

CAS–RN: 540–84–1
Group No.: 11–034
Molar Mass: 114.23

TABLE 11.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30PAR/HUF2	169.6–295.2	15	1.00	not specified		C_p	BSIO	25PAR
40PIT2	171.1–317.3	8	0.20	99.99	melpt	C_p	BSIO	28LAT/GRE
47OSB/GIN	285.6–305.6	5S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN
49TSC/WET	298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
50AUE/SAG	299.8–366.5	13	1.00	99.9	melpt	C_p	BSAO	39SAG/EVA
61ROU	300.4–315.4	12	nosp	99.99	anal	C_p	BSAO	61ROU
73SUB/RAJN	298.1–323.1	3	0.30	not specified		C_p	BSIO	64MOE/THO
76FOR/BEN1	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84FIL/LAU	293.0	1	2.00	not specified		C_p	BDHO	84FIL/LAU
87KAL/KOH	293.1–313.1	2	nosp	99.98	chrom	C_p	FSIT	71PIC/LED
88COS/VAN	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
88SHI/OGA1	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 11.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40PIT2	171.1–317.3	8	0.20	0.771	4.21–2	0.15	2.54–2	4
47OSB/GIN	285.6–305.6	5	0.10	0.545	1.54–2	0.05	–8.22–3	–2
50AUE/SAG	299.8–366.5	13	1.00	0.310	9.25–2	0.31	–8.23–2	–11
76FOR/BEN1	298.1	1	0.50#	0.265	3.81–2	0.13	3.81–2	1
84FIL/LAU	293.0	1	2.00	0.014	8.12–3	0.03	–8.12–3	–1
				Rejected data				
30PAR/HUF2	(2.62–1, 0.98, –2.35–1, –14)			49TSC/WET	(8.14–1, 2.92, –8.14–1, –1)			
61ROU	(1.35–1, 0.46, 7.33–2, 4)			73SUB/RAJ	(3.39–1, 1.15, –2.93–1, –3)			
87KAL/KOH	(5.71–1, 1.89, 4.93–1, 2)			88COS/VAN	(4.71–1, 1.62, 4.71–1, 1)			
88SHI/OGA1	(1.37–1, 0.47, 1.37–1, 1)							

TABLE 11.34.3. Parameters of regression polynomial

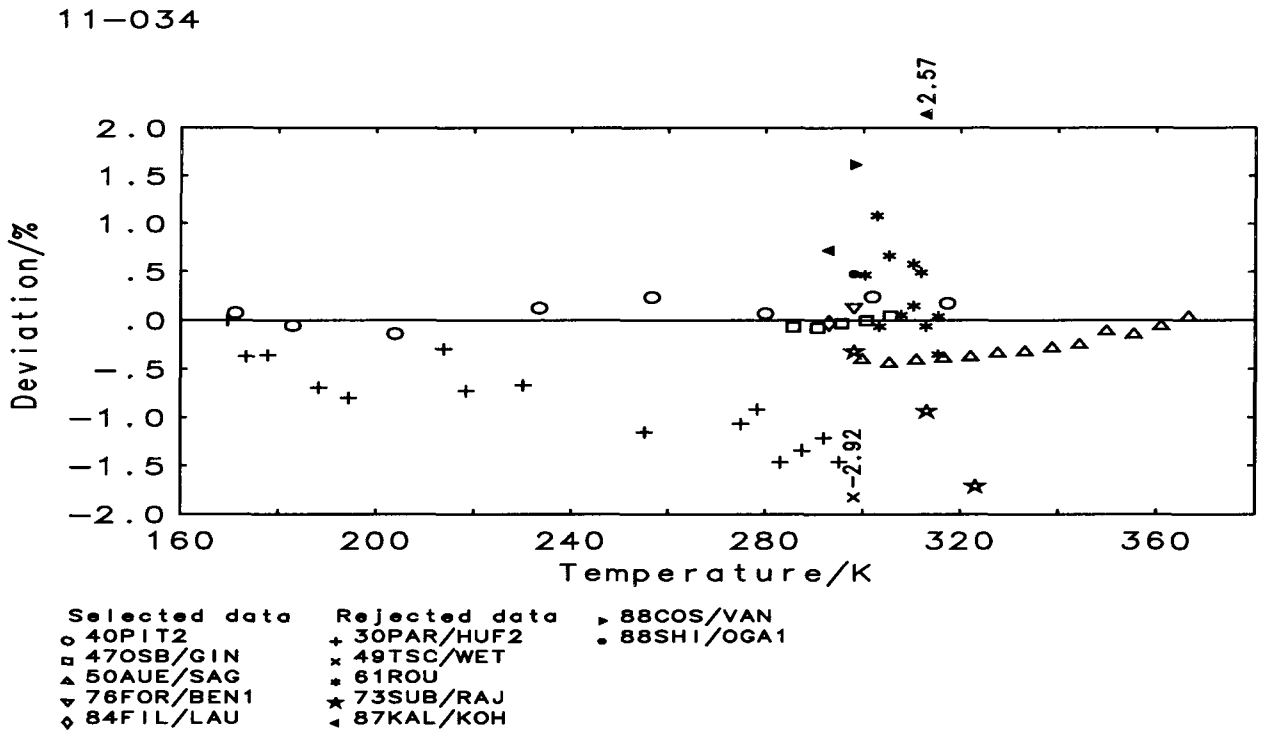
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	63	28	0.561	7.31–2	0.25	–3.14–2	–9
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
171.1–366.5	2.00353+1	–1.43004	1.91141	–1.53543–1			III

TABLE 11.34.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c ($J K^{-1} g^{-1}$)	1.629	1.657	1.686	1.717	1.750	1.784	1.819
C ($J K^{-1} mol^{-1}$)	186.0	189.2	192.6	196.2	199.9	203.8	207.8
Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1} g^{-1}$)	1.855	1.893	1.932	1.972	1.984	2.012	2.054
C ($J K^{-1} mol^{-1}$)	211.9	216.2	220.7	225.2	226.7	229.9	234.6
Temp. (K)	298.15	300	310	320	330	340	350
c ($J K^{-1} g^{-1}$)	2.089	2.096	2.140	2.184	2.228	2.273	2.319
C ($J K^{-1} mol^{-1}$)	238.6	239.5	244.4	249.4	254.5	259.7	264.9
Temp. (K)	360	370					
c ($J K^{-1} g^{-1}$)	2.365	2.412					
C ($J K^{-1} mol^{-1}$)	270.2	275.5					

TABLE 11.34.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	63	28	0.928	8.12–2	0.28	–3.23–2	–8
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
171.1–366.5	544.00	–6.41602	7.86779–1	1.46601+1	1.30804+1		III



Name: 2,3,3–Trimethylpentane
Formula: C_8H_{18}

CAS–RN: 560–21–4
Group No.: 11–035
Molar Mass: 114.23

TABLE 11.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47OSB/GIN	290.6–305.6	4	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN

TABLE 11.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	0.593	1.75–2	0.06	1.62–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
290.6–305.6		1.33968+2	–8.15968+1	1.56188+1			II

TABLE 11.35.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.088	2.149	2.165	2.265
C_{sat} (J K^{-1}mol^{-1})	238.6	245.5	247.3	258.7

Name: 2,3,4–Trimethylpentane
Formula: C_8H_{18}

CAS–RN: 565–75–3
Group No.: 11–036
Molar Mass: 114.23

TABLE 11.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41PIT/SCO	172.8–323.6	14	0.20	99.75	melpt	C_p	BSIO	28LAT/GRE
47OSB/GIN	290.6–305.6	4S	0.10	99.96	melpt	C_{sat}	BSAO	47OSB/GIN

TABLE 11.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41PIT/SCO	172.8–323.6	14	0.70#	1.534	3.20–1	1.07	1.67–2	2
47OSB/GIN	290.6–305.6	4	0.20#	3.399	2.03–1	0.68	–7.15–5	0

TABLE 11.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	18	18	2.378	3.38–1	1.13	1.30–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
172.8–323.6	–1.39272+1	4.42905+1	–1.79226+1	2.67701	IV

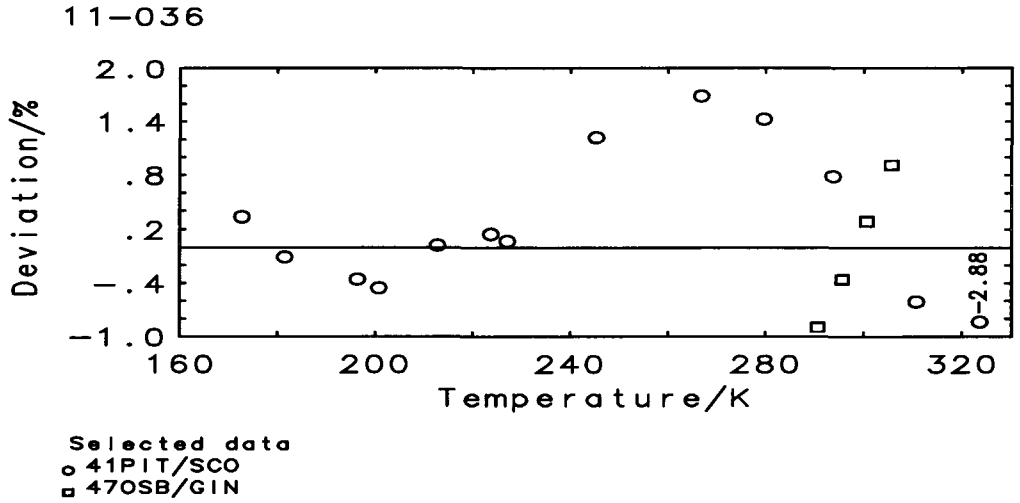
TABLE 11.36.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c ($J K^{-1} g^{-1}$)	1.654	1.699	1.739	1.775	1.808	1.839	1.871
C ($J K^{-1} mol^{-1}$)	188.9	194.1	198.6	202.7	206.5	210.1	213.7
Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1} g^{-1}$)	1.903	1.937	1.974	2.016	2.030	2.063	2.116
C ($J K^{-1} mol^{-1}$)	217.4	221.3	225.5	230.3	231.9	235.6	241.8
Temp. (K)	298.15	300	310	320			
c ($J K^{-1} g^{-1}$)	2.166	2.178	2.248	2.329			
C ($J K^{-1} mol^{-1}$)	247.4	248.8	256.8	266.0			

TABLE 11.36.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	18	18	3.456	2.15–1	0.75	–7.21–2	–1 0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
172.8–323.6	566.30	–7.64507	9.15039–1	1.39061+1	1.59685+1	IV



Name: 3,3–Diethylpentane
Formula: C_9H_{20}

CAS–RN: 1067–20–5
Group No.: 11–037
Molar Mass: 128.26

TABLE 11.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54STA/WAR	250.0–260.0	2S	0.50	99.50	melpt	C_p	BSAO	49STA/GUP
76FIN/MES	243.2–365.4	16	0.20	99.985	melpt	C_{sat}	BSAO	43RUE/HUF
79FUC/PEA	298.1	1	nosp	99.	chrom	C_p	BSIO	80FUC

TABLE 11.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76FIN/MES	243.2–365.4	16	0.20#	0.384	2.57–2	0.08	5.18–4	–1
79FUC/PEA	298.1	1	0.50#	0.287	4.80–2	0.14	–4.80–2	–1
				Rejected data				
54STA/WAR	(5.71–1, 1.84, 5.71–1, 2)							

TABLE 11.37.3. Parameters of regression polynomial

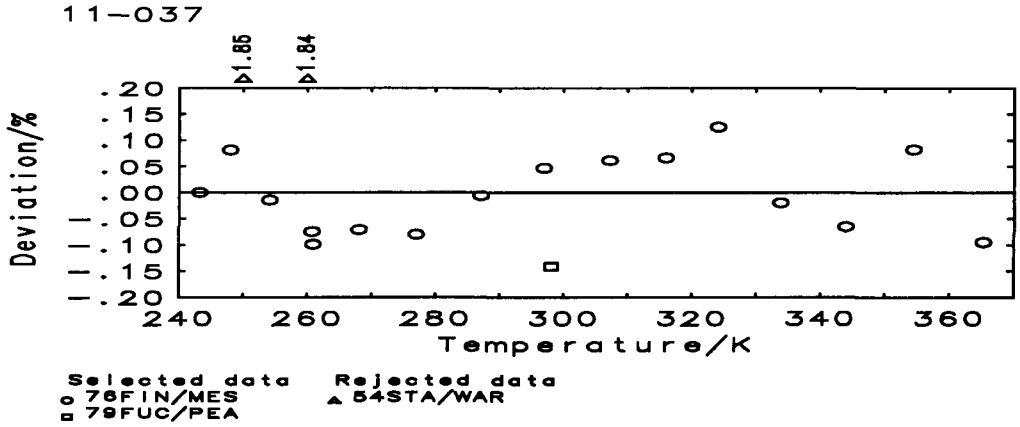
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	19	17	0.418	3.04–2	0.09	–2.34–3	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
243.2–365.4		1.45855+1	5.47668	2.92227–1			II

TABLE 11.37.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c ($J K^{-1}g^{-1}$)	1.952	1.997	2.042	2.057	2.088	2.134	2.172
C ($J K^{-1}mol^{-1}$)	250.3	256.1	261.9	263.8	267.8	273.8	278.6
Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1}g^{-1}$)	2.181	2.228	2.276	2.323	2.372	2.420	2.469
C ($J K^{-1}mol^{-1}$)	279.7	285.8	291.9	298.0	304.2	310.4	316.7
Temp. (K)	370						
c ($J K^{-1}g^{-1}$)	2.518						
C ($J K^{-1}mol^{-1}$)	323.0						

TABLE 11.37.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	19	17	0.479	3.47–2	0.10	–3.33–3	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
243.2–365.4	616.00	–5.83313	2.64844–1	1.35863+1	3.21184+1		II



Name: Nonane
Formula: C_9H_{20}

CAS-RN: 111–84–2
Group No.: 11–038
Molar Mass: 128.26

TABLE 11.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF2		224.5–299.1	8	1.00	not specified		C_p	BSIO	25PAR
31HUF/PAR		228.3–297.9	8	1.00	not specified		C_p	BSIO	25PAR
47OSB/GIN		283.1–313.1	4S	0.10	99.96	estim	C_{sat}	BSAO	47OSB/GIN
54FIN/GRO2	N	225.0–313.9	22	0.20	99.88	melpt	C_{sat}	BSAO	43RUE/HUF
58SWI/ZIE1	N	348.8	1	nosp	not specified		avg	DSIO	58SWI/ZIE1
70AKH		293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS
76MUS		307.8–417.8	10	2.50	not specified		C_p	BDAO	71MUS
79GRO/HAM		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
82WIL/ING		298.1	1	nosp	99.0	estim	C_p	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	99.8	chrom	C_p	BDCT	91BAN/GAR
91OGA/MIT		298.1	1	nosp	not specified		C_p	FSIO	85OGA
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

54FIN/GRO2 smoothed data in 67MES/GUT
58SWI/ZIE1 average value in temperature range 295–402 K

TABLE 11.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47OSB/GIN	283.1–313.1	4	0.10	1.657	5.66–2	0.17	2.37–3	0
54FIN/GRO2	225.0–313.9	22	0.20	0.305	2.04–2	0.06	5.40–3	2
79GRO/HAM	298.1	1	0.50#	0.282	4.82–2	0.14	–4.82–2	–1
82WIL/ING	298.1	1	0.50#	0.494	8.43–2	0.25	–8.43–2	–1
88AND/PAT	298.1	1	0.50#	0.224	3.84–2	0.11	3.84–2	1
91BAN/GAR	318.1–373.1	12	0.40#	0.564	8.16–2	0.23	–4.50–2	–7
91TRE/COS	298.1	1	0.50#	0.071	1.22–2	0.04	–1.22–2	–1
				Rejected data				
30PAR/HUF2	(4.25–1, 1.29, –4.24–1, –7)			31HUF/PAR	(3.05–1, 0.93, –2.99–1, –8)			
58SWI/ZIE1	(1.62, 4.18, 1.62, 1)			70AKH	(5.79–1, 1.68, 5.79–1, 1)			
76MUS	(9.12–1, 2.47, –8.09–1, –6)			91OGA/MIT	(2.04–1, 0.59, 2.04–1, 1)			

TABLE 11.38.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	71	42	0.683	5.53–2	0.16	–1.23–2	–7
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
225.0–300.0	1.23077+2	–1.00722+2	3.58380+1	–4.04253			II
300.0–373.1	–8.26076+1	1.04963+2	–3.27236+1	3.57543			III

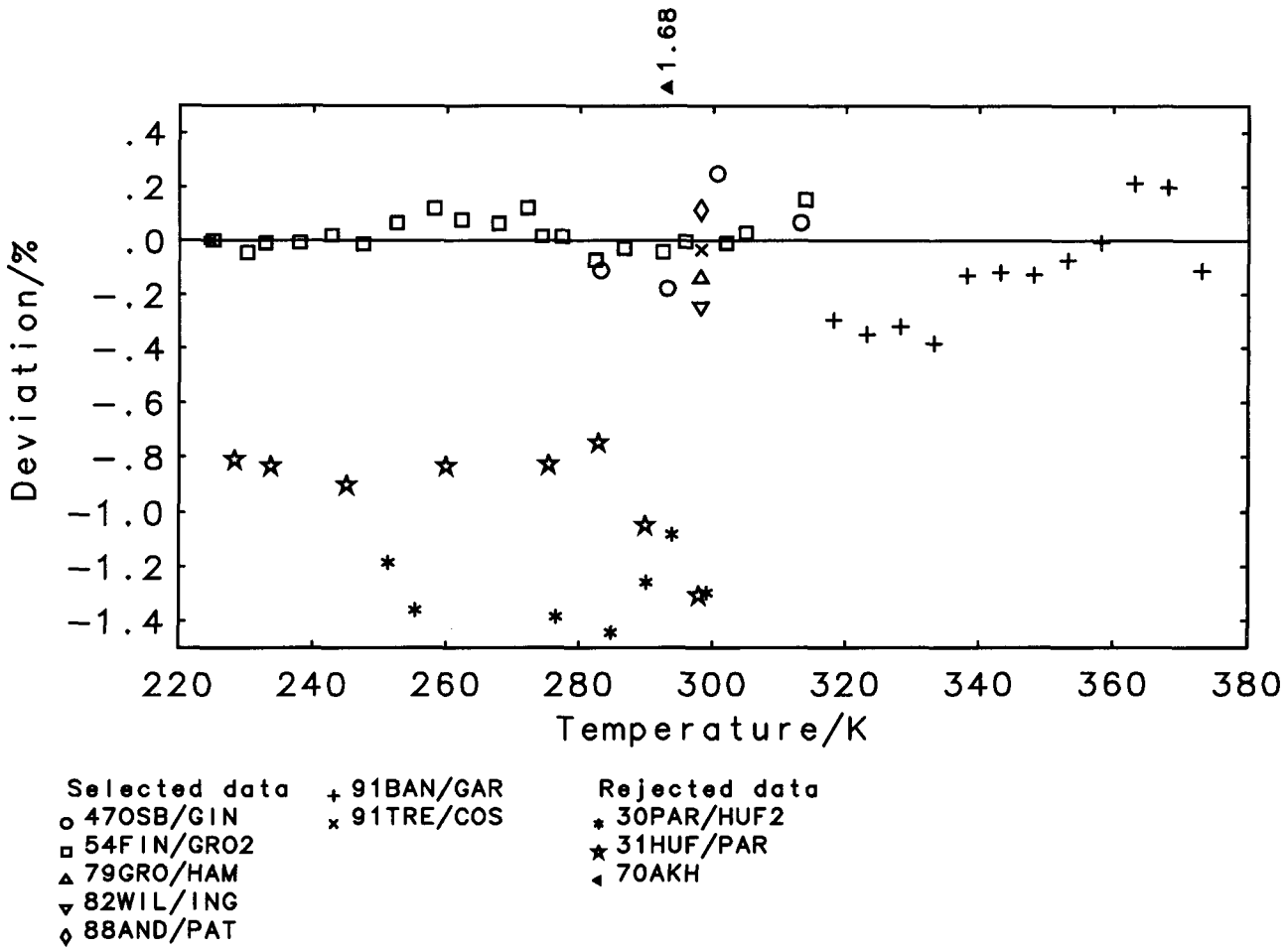
TABLE 11.38.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.062	2.067	2.081	2.101	2.128	2.137	2.158
C_p (J K^{-1}mol^{-1})	264.5	265.1	266.9	269.5	272.9	274.0	276.7
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.190	2.218	2.224	2.257	2.291	2.327	2.367
C_p (J K^{-1}mol^{-1})	280.9	284.4	285.2	289.5	293.9	298.5	303.6
Temp. (K)	350	360	370				
c_p (J K^{-1}g^{-1})	2.411	2.462	2.520				
C_p (J K^{-1}mol^{-1})	309.3	315.8	323.2				

TABLE 11.38.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	71	41	1.618	9.62–2	0.28	–7.53–3	–8

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
230.1–373.1	594.90	1.14187+1	1.20016+1	1.66310+1	2.71605	III



Name: 2,2,3,3-Tetramethylpentane
Formula: C_9H_{20}

CAS-RN: 7154-79-2
Group No.: 11-039
Molar Mass: 128.26

TABLE 11.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76FIN/MES	269.2–392.7	19	0.20	99.993	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 11.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	19	19	0.225	1.57-2	0.04	1.28-5	-1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
269.2–392.7		1.26743+1	6.40507	9.95780-2			II

TABLE 11.39.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.990	2.004	2.035	2.080	2.117	2.125	2.171
C_{sat} (J K^{-1}mol^{-1})	255.2	257.0	261.0	266.8	271.5	272.6	278.4
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.216	2.262	2.308	2.354	2.400	2.446	2.493
C_{sat} (J K^{-1}mol^{-1})	284.3	290.1	296.0	301.9	307.8	313.8	319.7
Temp. (K)	390						
c_{sat} (J K^{-1}g^{-1})	2.539						
C_{sat} (J K^{-1}mol^{-1})	325.7						

TABLE 11.39.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.222	1.56–2	0.04	1.15–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
269.2–392.7	607.60	–1.47040	1.36537–2	1.22125+1	3.95878+1		II

Name: 2,2,4,4–Tetramethylpentane
Formula: C_9H_{20}

CAS–RN: 1070–87–7
Group No.: 11–040
Molar Mass: 128.26

TABLE 11.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76FIN/MES	212.7–379.5	19	0.20	99.985	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 11.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.253	1.65–2	0.05	1.31–5	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
212.7–379.5		2.11552+1	–1.50750	2.34209	–2.05882–1		II

TABLE 11.40.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.712	1.749	1.787	1.827	1.867	1.909	1.952
C_{sat} (J K^{-1}mol^{-1})	219.6	224.3	229.3	234.3	239.5	244.9	250.3
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.965	1.995	2.039	2.076	2.084	2.130	2.176
C_{sat} (J K^{-1}mol^{-1})	252.1	255.9	261.6	266.3	267.3	273.2	279.1
Temp. (K)	330	340	350	360	370	380	
c_{sat} (J K^{-1}g^{-1})	2.223	2.270	2.317	2.365	2.412	2.460	
C_{sat} (J K^{-1}mol^{-1})	285.1	291.1	297.2	303.3	309.4	315.5	

TABLE 11.40.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.638	4.08–2	0.13	1.09–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
212.7–379.5	574.70	–6.23952	3.98970–1	1.39685+1	2.43951+1		II

Name: Decane
Formula: $C_{10}H_{22}$

CAS–RN: 124–18–5
Group No.: 11–041
Molar Mass: 142.28

TABLE 11.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*98LOU	N	360.9	1	nosp	not specified	avg	DSIO	*98LOU
30PAR/HUF2		242.3–295.5	6	1.00	not specified	C_p	BSIO	25PAR
31HUF/PAR		251.2–297.7	6	1.00	not specified	C_p	BSIO	25PAR
47OSB/GIN		290.6–305.6	4S	0.10	99.96 estim	C_{sat}	BSAO	47OSB/GIN
52SCH/SAG		299.8–366.5	13S	1.00	99.7 estim	C_{sat}	BSAO	39SAG/EVA
54FIN/GRO2	N	247.0–318.6	17	0.20	99.91 melpt	C_{sat}	BSAO	43RUE/HUF
70AKH		293.1	1	nosp	not specified	C_p	BDHO	59ABA/MUS
75GRI/RAS	N	303.3–462.4	9	1.00	not specified	C_p	BDAO	75RAS/GRI
79GRO/HAM		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
82WIL/ING		298.1	1	nosp	99.0 estim	C_p	FSIT	71PIC/LED
83SID/SVE		293.1	1	nosp	99.9 melpt	C_p	FSIT	71PIC/LED
84GRO/ING		298.1	1	nosp	99.0 melpt	C_p	FSIT	71PIC/LED
84ROU/GRO		298.1	1	nosp	98.0 estim	C_p	FSIT	71PIC/LED
85BAL/BRA		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
85COS/PAT3		298.2	1	nosp	99. anal	C_p	FSIT	71PIC/LED
85COS/PAT8		283.1–313.1	3	nosp	99. estim	C_p	FSIT	71PIC/LED
85LAI/ROD		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
85LAI/WIL		298.1	1	0.30	99. estim	C_p	FSIT	71PIC/LED
86GAT/WOO		298.1–368.1	4	nosp	99. anal	C_p	BDCT	83ROU/ROU
87WIL/ING		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
88KUZ/KHA		293.8–335.2	15	nosp	99.8 chrom	C_p	FSIO	75SAF/GER
88KUZ/KHA		310.1–421.9	16	nosp	not specified	C_p	BSAO	67RAS/GAN
88PIN/BRA		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	98.9 chrom	C_p	BDCT	91BAN/GAR
91TRE/COS		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED

*98LOU average value in temperature range 295–427 K
54FIN/GRO2 smoothed data in 67MES/GUT
75GRI/RAS last two values at pressures above the vapour pressure

TABLE 11.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	247.0–318.6	17	0.20	0.158	1.17–2	0.03	–1.09–4	–2
75GRI/RAS	303.3–462.4	9	1.00	0.667	2.77–1	0.67	–7.66–2	–1
84GRO/ING	298.1	1	0.50#	0.310	5.84–2	0.15	–5.84–2	–1
84ROU/GRO	298.1	1	0.50#	0.131	2.47–2	0.07	–2.47–2	–1
86GAT/WOO	298.1–368.1	4	0.30#	1.126	1.36–1	0.34	–1.35–1	–4
88KUZ/KHA	293.8–335.2	15	0.50#	0.419	8.04–2	0.21	7.32–2	15
88KUZ/KHA	310.1–421.9	16	0.60#	0.330	8.54–2	0.20	3.50–2	4
91BAN/GAR	318.1–373.1	12	0.40	0.327	5.50–2	0.13	1.64–2	1
				Rejected data				
*98LOU	(3.97–1, 0.94, 3.97–1, 1)				30PAR/HUF2	(6.60–1, 1.85, –6.22–1, –5)		
31HUF/PAR	(3.10–1, 0.85, –3.06–1, –6)				47OSB/GIN	(3.28–1, 0.87, –2.70–2, 0)		
52SCH/SAG	(4.05–1, 1.04, –3.67–1, –11)				70AKH	(4.51–1, 1.22, –4.51–1, –1)		
79GRO/HAM	(1.34–1, 0.36, –1.34–1, –1)				82WIL/ING	(2.28–1, 0.61, –2.28–1, –1)		
83SID/SVE	(2.26–1, 0.61, –2.26–1, –1)				85BAL/BRA	(1.41–1, 0.38, –1.41–1, –1)		
85COS/PAT3	(1.23–1, 0.32, 1.23–1, 1)				85COS/PAT8	(1.55–1, 0.40, 4.26–2, 1)		
85LAI/ROD	(1.71–1, 0.46, –1.71–1, –1)				85LAI/WIL	(1.60–1, 0.42, –1.60–1, –1)		
87WIL/ING	(1.80–1, 0.48, –1.80–1, –1)				88COS/VAN	(1.09–1, 0.29, 1.09–1, 1)		
88PIN/BRA	(1.55–1, 0.41, –1.55–1, –1)				91TRE/COS	(1.26–1, 0.33, 1.26–1, 1)		
92LAI/ROD	(2.18–1, 0.58, –2.18–1, –1)							

TABLE 11.41.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	121	75	0.467	1.21–1	0.29	7.22–3	11
C_{sat}	121	75	0.468	1.21–1	0.29	0.25–3	10
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
247.0–314.0		8.33283+1	–5.10491+1	1.70127+1	–1.68060		II
314.0–462.4		3.55264+1	–5.37839	2.46788	–1.36562–1		III
247.0–314.0		8.29151+1	–5.06122+1	1.68594+1	–1.66276		II
314.0–462.4		3.67462+1	–6.50171	2.81150	–1.71470–1		III

TABLE 11.41.4. Recommended values of heat capacities

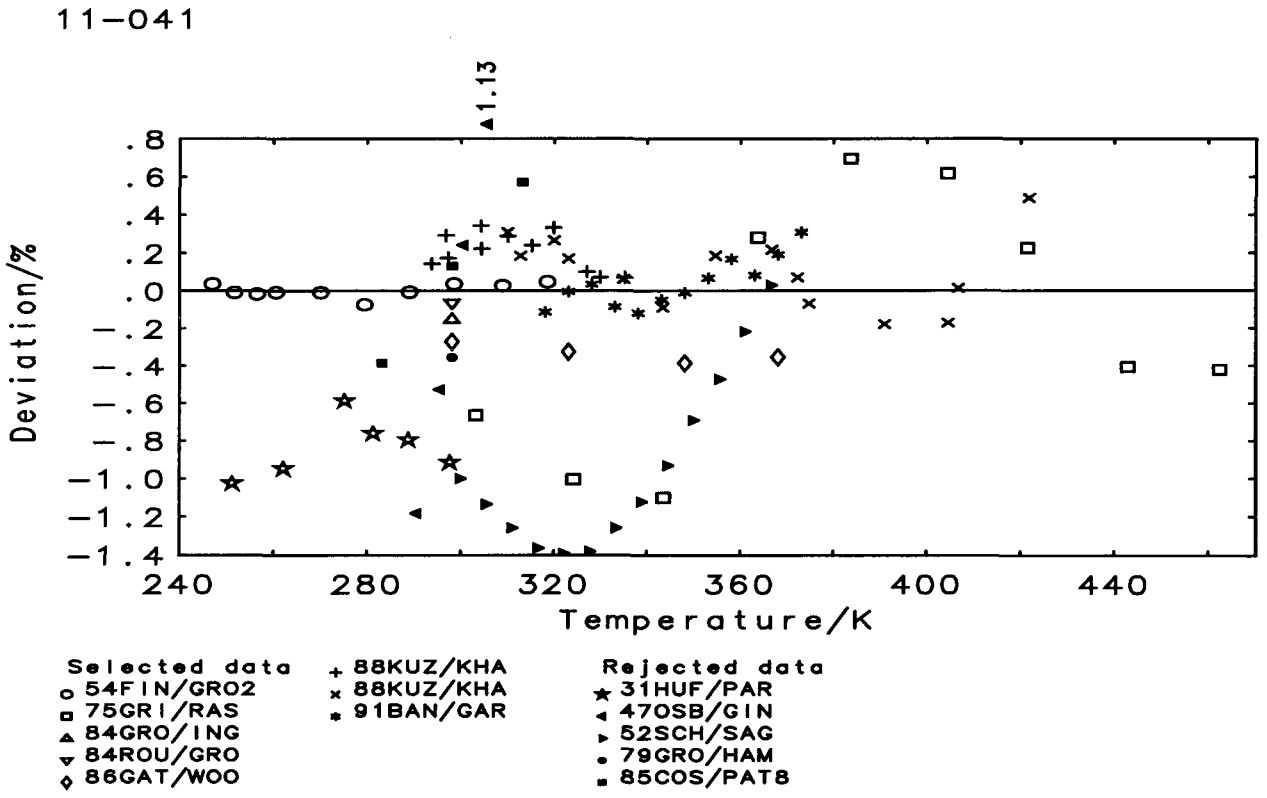
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	2.091	2.108	2.129	2.137	2.155	2.184	2.210
C_p ($J K^{-1} mol^{-1}$)	297.5	299.9	303.0	304.1	306.6	310.8	314.4
c_{sat} ($J K^{-1} g^{-1}$)	2.091	2.108	2.129	2.137	2.155	2.184	2.210
C_{sat} ($J K^{-1} mol^{-1}$)	297.5	299.9	303.0	304.1	306.6	310.8	314.4
Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1} g^{-1}$)	2.216	2.250	2.286	2.323	2.361	2.400	2.441
C_p ($J K^{-1} mol^{-1}$)	315.3	320.1	325.2	330.5	335.9	341.5	347.4
c_{sat} ($J K^{-1} g^{-1}$)	2.216	2.250	2.286	2.323	2.361	2.400	2.441
C_{sat} ($J K^{-1} mol^{-1}$)	315.3	320.1	325.2	330.5	335.9	341.6	347.4

TABLE 11.41.4. Recommended values of heat capacities—Continued

Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1}g^{-1}$)	2.483	2.526	2.570	2.616	2.662	2.709	2.757
C_p ($J K^{-1}mol^{-1}$)	353.3	359.4	365.7	372.1	378.7	385.4	392.2
c_{sat} ($J K^{-1}g^{-1}$)	2.483	2.526	2.570	2.615	2.661	2.707	2.755
C_{sat} ($J K^{-1}mol^{-1}$)	353.3	359.4	365.7	372.1	378.6	385.2	391.9
Temp. (K)	440	450	460				
c_p ($J K^{-1}g^{-1}$)	2.805	2.855	2.905				
C_p ($J K^{-1}mol^{-1}$)	399.2	406.2	413.3				
c_{sat} ($J K^{-1}g^{-1}$)	2.803	2.851	2.901				
C_{sat} ($J K^{-1}mol^{-1}$)	398.8	405.7	412.7				

TABLE 11.41.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	121	75	1.223	2.15–1	0.51	3.02–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
247.0–462.4	617.65	–8.49622	1.93863	2.41305+1	9.30887		III



Name: 2,7–Dimethyloctane
Formula: $C_{10}H_{22}$

CAS–RN: 1072–16–8
Group No.: 11–042
Molar Mass: 142.28

TABLE 11.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30PAR/HUF2	223.2–295.0	8	1.00	not specified		C_p	BSIO	25PAR

TABLE 11.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.194	6.70–2	0.19	2.19–4	0
Temp. range K		A_1	A_2				Level of uncertainty
223.2–295.0		2.03020+1	5.40560				IV

TABLE 11.42.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.913	1.944	1.976	2.008	2.039	2.049	2.071
C_p (J K^{-1}mol^{-1})	272.2	276.7	281.2	285.7	290.2	291.6	294.6
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	2.102	2.128	2.134				
C_p (J K^{-1}mol^{-1})	299.1	302.8	303.6				

Name: 2–Methylnonane
Formula: $C_{10}H_{22}$

CAS–RN: 871–83–0
Group No.: 11–043
Molar Mass: 142.28

TABLE 11.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41PAR/WES	200.0–298.0	11S	0.25	99.1	melpt	C_p	BSIO	25PAR

TABLE 11.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.258	2.22–2	0.06	2.32–5	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.0–298.0		7.94595+1	–5.37085+1	1.95595+1	–2.09386		III

TABLE 11.43.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.959	1.960	1.968	1.982	2.003	2.029	2.059
C_p (J K^{-1}mol^{-1})	278.8	278.9	280.0	282.1	285.0	288.7	293.0
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	2.093	2.105	2.130	2.170	2.203	2.211	
C_p (J K^{-1}mol^{-1})	297.8	299.5	303.1	308.7	313.5	314.6	

TABLE 11.43.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	1.205	1.06–1	0.30	4.30–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.0–298.0	609.30	2.05696+2	8.86112+1	–5.58771+1	1.19373+2		III

Name: 3–Methylnonane
Formula: $C_{10}H_{22}$

CAS–RN: 5911–04–6
Group No.: 11–044
Molar Mass: 142.28

TABLE 11.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41PAR/WES	N	190.0–298.0	12S	0.25	99.7	melpt	C_p	BSIO	25PAR

41PAR/WES racemic mixture

TABLE 11.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.548	4.67–2	0.14	9.46–5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
190.0–298.0	3.38710+1	–5.08070	2.08079	III

TABLE 11.44.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.854	1.872	1.892	1.915	1.940	1.967	1.997
C_p (J K^{-1}mol^{-1})	263.8	266.3	269.2	272.4	276.0	279.9	284.1
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.029	2.064	2.076	2.101	2.141	2.175	2.183
C_p (J K^{-1}mol^{-1})	288.7	293.7	295.3	299.0	304.6	309.5	310.6

TABLE 11.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.624	5.47–2	0.16	1.19–4	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
190.0–298.0	613.70	2.77878+1	2.49312+1	3.48471	7.74292	III

Name: 4–Methylnonane
Formula: $C_{10}H_{22}$

CAS–RN: 17301–94–9
Group No.: 11–045
Molar Mass: 142.28

TABLE 11.45.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41PAR/WES	N	180.0–298.0	13S	0.25	99.3	melpt	C_p	BSIO	25PAR

41PAR/WES racemic mixture

TABLE 11.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.666	5.39–2	0.17	1.31–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
180.0–298.0		3.55303+1	–6.71178	2.54999			II

TABLE 11.45.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.853	1.869	1.888	1.910	1.935	1.962	1.993
C_p (J K^{-1}mol^{-1})	263.7	265.9	268.6	271.7	275.3	279.2	283.6
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.027	2.064	2.104	2.117	2.146	2.192	2.231
C_p (J K^{-1}mol^{-1})	288.4	293.6	299.3	301.2	305.4	311.9	317.5
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	2.241						
C_p (J K^{-1}mol^{-1})	318.8						

TABLE 11.45.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.834	6.84–2	0.21	2.07–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
180.0–298.0	613.70	5.02490+1	3.62593+1	–7.31356	1.74091+1		III

Name: 5–Methylnonane
Formula: $C_{10}H_{22}$

CAS–RN: 15869–85–9
Group No.: 11–046
Molar Mass: 142.28

TABLE 11.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
41PAR/WES	190.0–298.0	12S	0.25	99.7	melpt	C_p	BSIO	25PAR

TABLE 11.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.221	1.97–2	0.06	1.19–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
190.0–298.0		3.47624+1	–6.04279	2.37084			III

TABLE 11.46.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.861	1.879	1.901	1.925	1.952	1.982	2.014
C_p (J K^{-1}mol^{-1})	264.7	267.4	270.5	273.9	277.8	282.0	286.6
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.050	2.088	2.101	2.129	2.172	2.210	2.219
C_p (J K^{-1}mol^{-1})	291.7	297.1	298.9	302.9	309.1	314.5	315.7

TABLE 11.46.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.426	3.67–2	0.11	5.26–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
190.0–298.0	613.70	3.59812+1	2.96818+1	–1.23427	1.09044+1		III

Name: 2–Methyldecane
Formula: $C_{11}H_{24}$

CAS–RN: 6975–98–0
Group No.: 11–047
Molar Mass: 156.31

TABLE 11.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71MES/FIN	235.4–384.8	22	0.20	99.979	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 11.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.342	2.91–2	0.07	2.51–5	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
235.4–384.8		5.68879+1	–2.46238+1	8.88342	–8.08008–1		II

TABLE 11.47.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.990	2.010	2.033	2.059	2.088	2.098	2.120
C_{sat} (J K^{-1}mol^{-1})	311.1	314.2	317.8	321.9	326.4	327.9	331.3
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	2.153	2.182	2.189	2.226	2.265	2.305	2.346
C_{sat} (J K^{-1}mol^{-1})	336.6	341.1	342.1	348.0	354.0	360.3	366.7
Temp. (K)	350	360	370	380			
c_{sat} (J K^{-1}g^{-1})	2.387	2.429	2.472	2.514			
C_{sat} (J K^{-1}mol^{-1})	373.2	379.7	386.3	392.9			

TABLE 11.47.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	1.158	9.43–2	0.23	3.66–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
235.4–384.8	623.00	–9.83062	4.11511	2.39812+1	5.87111		II

Name: Undecane
Formula: $C_{11}H_{24}$

CAS–RN: 1120–21–4
Group No.: 11–048
Molar Mass: 156.31

TABLE 11.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31HUF/PAR		258.5–298.0	4	1.00	not specified		C_p	BSIO	25PAR
54FIN/GRO2	N	251.7–298.9	12	0.20	99.98	melpt	C_{sat}	BSAO	43RUE/HUF
70AKH		293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS
76MUS		307.8–458.6	14	2.50	not specified		C_p	BDAO	71MUS
84GRI/AND		292.3–433.4	8	0.80	not specified		C_p	BSAO	67RAS/GAN

54FIN/GRO2 smoothed data in 67MES/GUT

TABLE 11.48.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	251.7–298.9	12	0.20	0.127	1.04–2	0.03	1.24–3	1
84GRI/AND	292.3–433.4	8	0.80	0.257	8.81–2	0.21	–2.92–2	0
				Rejected data				
31HUF/PAR	(1.96–1, 0.48, –1.87–1, –4)			70AKH	(4.84–1, 1.16, 4.84–1, 1)			
76MUS	(3.05, 6.87, –2.94, –11)							

TABLE 11.48.3. Parameters of cubic spline polynomials

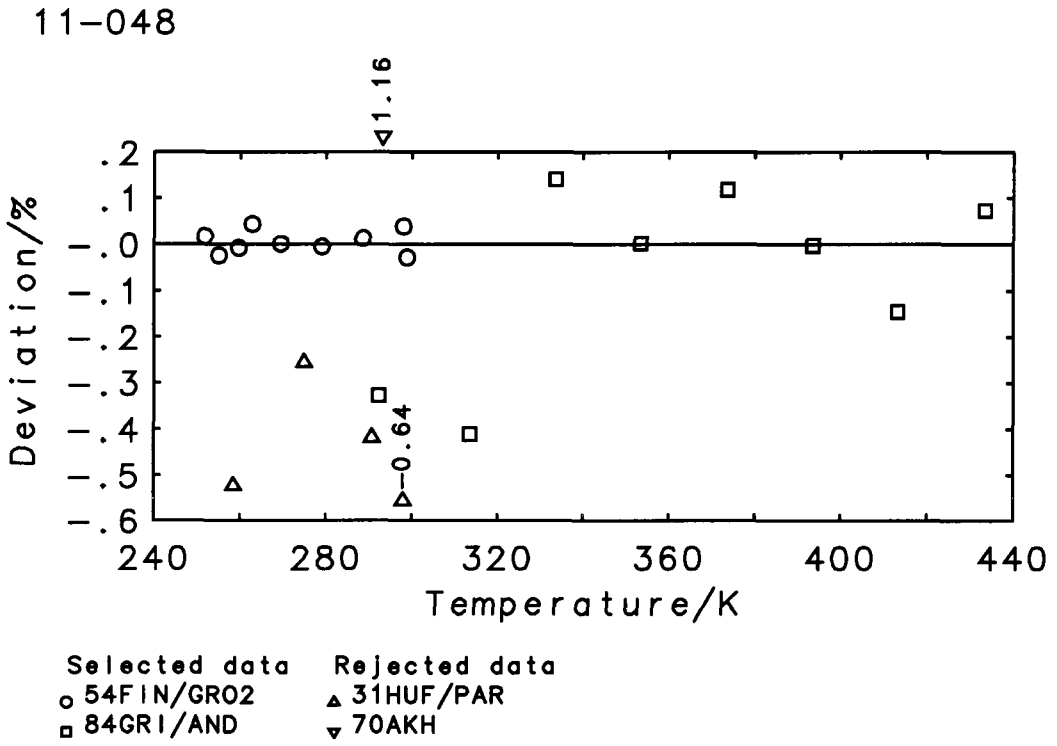
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	20	0.220	6.50–2	0.15	–1.09–2	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
251.7–300.0		1.64553+2	–1.29722+2	4.35318+1	–4.65086		II
300.0–433.4		5.51273+1	–2.02967+1	7.05661	–5.98064–1		IV

TABLE 11.48.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	2.109	2.117	2.133	2.140	2.156	2.183	2.207
C_p ($J K^{-1} mol^{-1}$)	329.7	331.0	333.5	334.5	336.9	341.2	345.0
Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1} g^{-1}$)	2.213	2.245	2.279	2.314	2.350	2.388	2.426
C_p ($J K^{-1} mol^{-1}$)	345.9	350.9	356.2	361.7	367.4	373.2	379.2
Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1} g^{-1}$)	2.465	2.504	2.544	2.584	2.623	2.662	2.701
C_p ($J K^{-1} mol^{-1}$)	385.3	391.5	397.6	403.8	410.0	416.1	422.2

TABLE 11.48.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	20	1.284	3.59–1	0.77	8.58–2	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
251.7–433.4	638.85	–7.00457–1	8.14112	2.56974+1	1.50667–2		V



Name: Dodecane
Formula: $C_{12}H_{26}$

CAS–RN: 112–40–3
Group No.: 11–049
Molar Mass: 170.34

TABLE 11.49.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31HUF/PAR		275.1–297.7	4	1.00	not specified		C_p	BSIO	25PAR
54FIN/GRO2	N	266.7–317.4	11	0.20	99.93	melpt	C_{sat}	BSAO	43RUE/HUF
71REC/SAD		303.1	1	0.30	not specified		C_p	BSIO	70REC
73KAL/WOY		303.1	1	0.20	99.5	chrom	C_p	BSIO	70REC
77NAZ/MUS		303.2–483.2	10	1.50	not specified		C_p	BSAO	77NAZ/MUS
81GRO/ING		298.1	1	nosp	99.0	chrom	C_p	FSIT	71PIC/LED
84GRO/BEN		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84KUM/BEN		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
84ROU/GRO		298.1	1	nosp	98.	estim	C_p	FSIT	71PIC/LED
85COS/PAT4		298.2	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
85COS/PAT8		283.1–313.1	3	nosp	99.0	estim	C_p	FSIT	71PIC/LED
85LAI/ROD		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
86BEN/DAR3		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
86WIL/LAI		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
89VOG/SCH		333.1	1	nosp	not specified		C_p	BDHT	69PER/COM
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

54FIN/GRO2 smoothed data in 67MES/GUT

TABLE 11.49.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	266.7–317.4	11	0.20	0.169	1.49–2	0.03	1.40–3	3
77NAZ/MUS	303.2–483.2	10	1.50	0.108	8.03–2	0.16	9.02–3	2
84GRO/BEN	298.1	1	0.50#	0.343	7.74–2	0.17	–7.74–2	–1
84KUM/BEN	298.1	1	0.50#	0.322	7.26–2	0.16	–7.26–2	–1
85COS/PAT4	298.2	1	0.50#	0.038	8.65–3	0.02	8.65–3	1
86BEN/DAR3	298.1	1	0.50#	0.284	6.41–2	0.14	–6.41–2	–1
88AND/PAT	298.1	1	0.50#	0.296	6.70–2	0.15	6.70–2	1
88COS/VAN	298.1	1	0.50#	0.099	2.25–2	0.05	2.25–2	1
91TRE/COS	298.1	1	0.50#	0.051	1.16–2	0.03	1.16–2	1
				Rejected data				
31HUF/PAR	(3.87–1, 0.87, –3.77–1, –4)			71REC/SAD	(4.39–1, 0.97, –4.39–1, –1)			
73KAL/WOY	(9.29–1, 2.08, –9.29–1, –1)			81GRO/ING	(1.30–1, 0.29, –1.30–1, –1)			
84ROU/GRO	(1.17–1, 0.26, –1.17–1, –1)			85COS/PAT8	(2.21–1, 0.48, 7.63–2, 1)			
85LAI/ROD	(3.13–1, 0.70, –3.13–1, –1)			86WIL/LAI	(3.13–1, 0.70, –3.13–1, –1)			
89LAI/ROD	(4.55–1, 1.02, –4.55–1, –1)			89VOG/SCH	(1.27, 2.60, 1.27, 1)			
92LAI/ROD	(3.55–1, 0.79, –3.55–1, –1)							

TABLE 11.49.3. Parameters of cubic spline polynomials

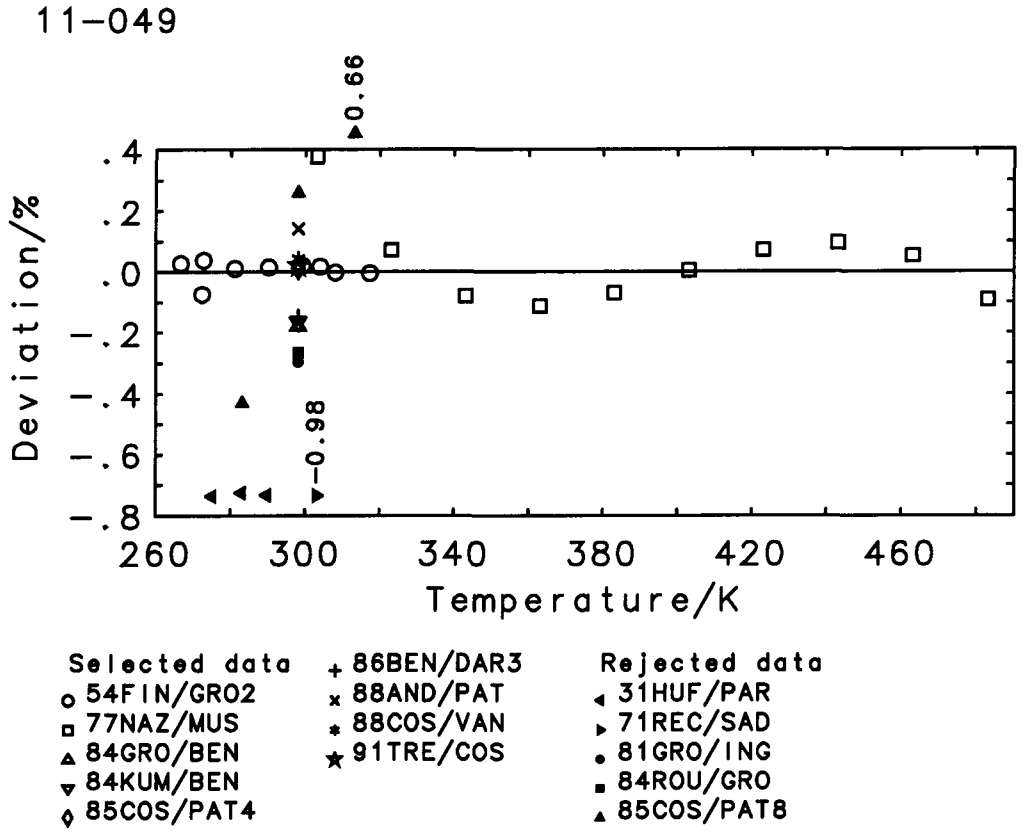
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	44	28	0.179	5.46–2	0.12	8.99–4	6
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
266.7–310.0		1.93881+2	–1.53376+2	5.06932+1	–5.35794		II
310.0–483.2		2.35104+1	1.14984+1	–2.49216	3.60918–1		IV

TABLE 11.49.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.141	2.146	2.160	2.184	2.207	2.212	2.243
C_p (J K^{-1}mol^{-1})	364.7	365.6	367.9	372.0	375.9	376.9	382.1
Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.275	2.308	2.342	2.377	2.414	2.451	2.490
C_p (J K^{-1}mol^{-1})	387.6	393.2	398.9	404.9	411.1	417.5	424.2
Temp. (K)	390	400	410	420	430	440	450
c_p (J K^{-1}g^{-1})	2.531	2.574	2.618	2.664	2.712	2.763	2.815
C_p (J K^{-1}mol^{-1})	431.2	438.4	446.0	453.8	462.0	470.6	479.5
Temp. (K)	460	470	480				
c_p (J K^{-1}g^{-1})	2.870	2.927	2.987				
C_p (J K^{-1}mol^{-1})	488.9	498.6	508.8				

TABLE 11.49.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	44	28	0.708	1.56–1	0.30	2.46–2	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
266.7–483.2	658.65	–1.01500+1	3.88605	2.90559+1	6.62768		IV



Name: 2,2,4,6,6–Pentamethylheptane
Formula: $C_{12}H_{26}$

CAS–RN: 13475–82–6
Group No.: 11–050
Molar Mass: 170.34

TABLE 11.50.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88COS/VAN	298.15	2.060	nosp	99.	anal	C_p	FSIT	71PIC/LED

Name: Tridecane
Formula: $C_{13}H_{28}$

CAS–RN: 629–50–5
Group No.: 11–051
Molar Mass: 184.37

TABLE 11.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54FIN/GRO2	N	271.7–306.4	8	0.20	99.95	melpt	C_{sat}	BSAO	43RUE/HUF
75WOY/KAL		303.1	1	nosp	99.97	chrom	C_p	BSIO	70REC
76MUS		307.8–478.6	16	2.50	not specified		C_p	BDAO	71MUS

54FIN/GRO2 smoothed data in 67MES/GUT

TABLE 11.51.2. Correlated heat capacities

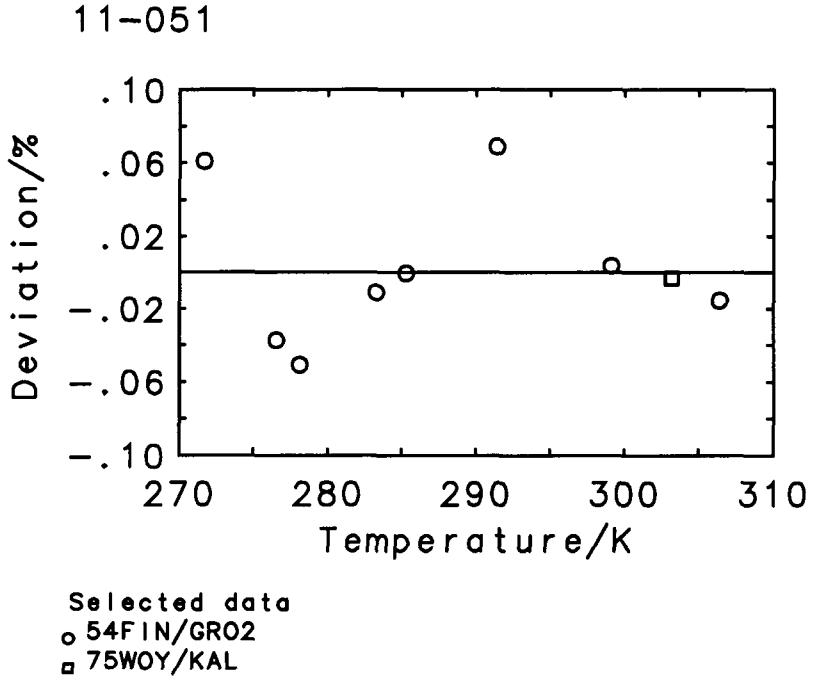
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	271.7–306.4	8	0.20	0.200	1.92–2	0.04	6.63–5	–2
75WOY/KAL	303.1	1	0.50#	0.011	2.59–3	0.01	–2.59–3	0

TABLE 11.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	25	9	0.231	2.23–2	0.05	–2.29–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
271.7–306.4		9.31514+1	–3.59261+1	7.07296			II

TABLE 11.51.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c ($J K^{-1} g^{-1}$)	2.152	2.155	2.165	2.185	2.206	2.211	2.244
C ($J K^{-1} mol^{-1}$)	396.7	397.4	399.2	402.8	406.7	407.7	413.7



Name: Tetradecane
Formula: $C_{14}H_{30}$

CAS-RN: 629-59-4
Group No.: 11-052
Molar Mass: 198.39

TABLE 11.52.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
34PAR/LIG		280.6–290.6	4	1.00	not specified		C_p	BSIO	25PAR
54FIN/GRO2	N	282.7–302.8	7	0.20	99.93	melpt	C_{sat}	BSAO	43RUE/HUF
76MUS		307.8–501.5	18	2.50	not specified		C_p	BDAO	71MUS
84GRI/AND		296.2–433.3	8	0.80	not specified		C_p	BSAO	67RAS/GAN
84GRO/BEN		298.1	1	nosp	99.5	estim	C_p	FSIT	71PIC/LED
84GRO/ING		298.1	1	nosp	99.	estim	C_p	FSIT	71PIC/LED
84ROU/GRO		298.1	1	nosp	99.	estim	C_p	FSIT	71PIC/LED
85BAL/BRA		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
85LAI/WIL		298.1	1	0.30	99.5	estim	C_p	FSIT	71PIC/LED
86WIL/LAI		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
87WIL/ING		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

54FIN/GRO2 smoothed data in 67MES/GUT

TABLE 11.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	282.7–302.8	7	0.20	0.158	1.67–2	0.03	8.95–3	2
84GRI/AND	296.2–433.3	8	0.80	0.344	1.53–1	0.28	–5.44–2	0
84ROU/GRO	298.1	1	0.50#	0.653	1.71–1	0.33	–1.71–1	–1
88COS/VAN	298.1	1	0.50#	0.149	3.92–2	0.07	–3.92–2	–1
91TRE/COS	298.1	1	0.50#	0.025	6.69–3	0.01	–6.69–3	–1
				Rejected data				
34PAR/LIG	(9.61–2, 0.18, –9.59–2, –3)			76MUS	(5.82, 10.99, –5.74, –11)			
84GRO/BEN	(2.33–1, 0.44, –2.33–1, –1)			84GRO/ING	(2.18–1, 0.42, –2.18–1, –1)			
85BAL/BRA	(5.78–1, 1.11, –5.78–1, –1)			85LAI/WIL	(4.97–1, 0.95, –4.97–1, –1)			
86WIL/LAI	(5.24–1, 1.00, –5.24–1, –1)			87WIL/ING	(5.02–1, 0.96, –5.02–1, –1)			
92LAI/ROD	(6.04–1, 1.16, –6.04–1, –1)							

TABLE 11.52.3. Parameters of cubic spline polynomials

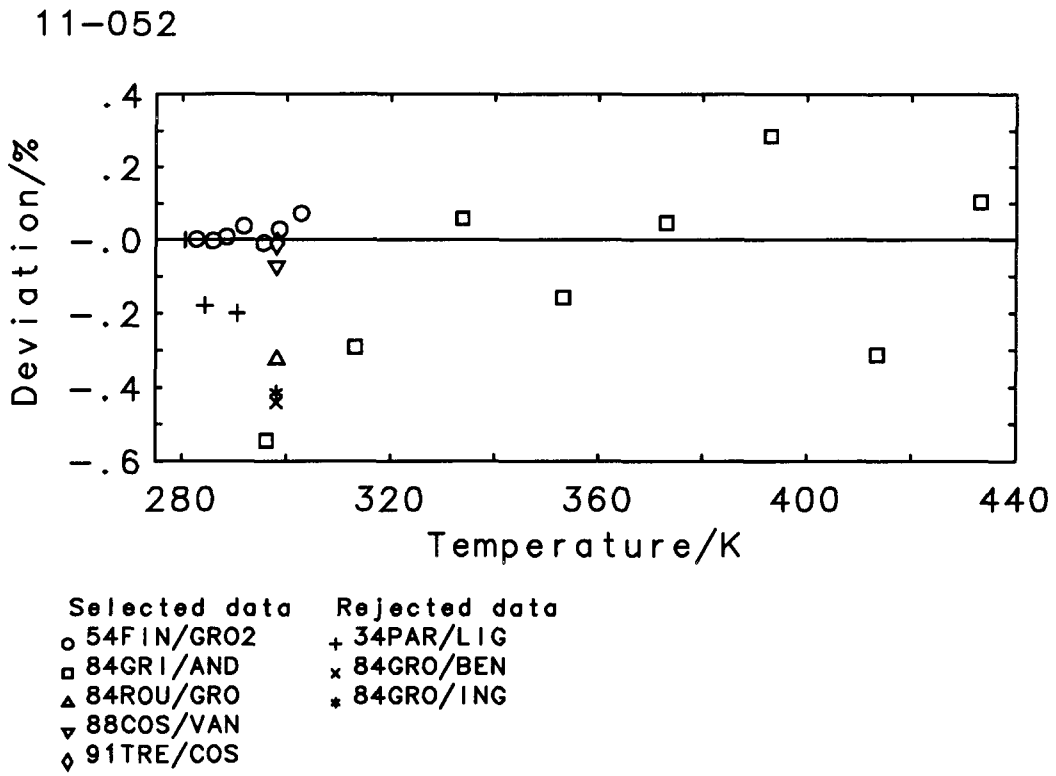
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	47	18	0.347	1.30–1	0.24	–3.28–2	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
282.7–310.0		1.43242+1	3.48980+1	–1.22889+1	1.64457		II
310.0–433.3		9.76193+1	–4.57102+1	1.37138+1	–1.15142		IV

TABLE 11.52.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	2.171	2.191	2.209	2.214	2.238	2.265	2.294
C_p ($J K^{-1} mol^{-1}$)	430.7	434.8	438.3	439.2	444.0	449.4	455.1
Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1} g^{-1}$)	2.325	2.358	2.392	2.427	2.463	2.499	2.536
C_p ($J K^{-1} mol^{-1}$)	461.3	467.8	474.5	481.5	488.6	495.8	503.1
Temp. (K)	410	420	430				
c_p ($J K^{-1} g^{-1}$)	2.572	2.608	2.644				
C_p ($J K^{-1} mol^{-1}$)	510.3	517.5	524.5				

TABLE 11.52.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	47	18	0.605	1.92–1	0.33	3.04–2	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
282.7–433.3	693.00	-8.99323	7.25409	3.37132+1	2.78733		IV



Name: Pentadecane
Formula: $C_{15}H_{32}$

CAS–RN: 629–62–9
Group No.: 11–053
Molar Mass: 212.42

TABLE 11.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
54FIN/GRO2	N	285.5–312.8	7	0.20	99.95	melpt	C_{sat}	BSAO	43RUE/HUF
70AKH		293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS
81GRO/ING		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

54FIN/GRO2 smoothed data in 67MES/GUT

TABLE 11.53.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	285.5–312.8	7	0.20	0.078	8.81–3	0.02	–1.37–3	–1
91TRE/COS	298.1	1	0.50#	0.214	6.05–2	0.11	6.05–2	1
				Rejected data				
70AKH	(7.09–1, 1.25, 7.09–1, 1)			81GRO/ING	(2.61–1, 0.46, –2.61–1, –1)			
88COS/VAN	(1.40–1, 0.25, –1.40–1, –1)							

TABLE 11.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	11	8	0.133	2.90–2	0.05	6.36–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
285.5–312.8		1.00964+2	–3.53605+1	6.86082			II

TABLE 11.53.4. *Recommended values of heat capacities*

Temp. (K)	280	290	298.15	300	310
c ($J K^{-1} g^{-1}$)	2.182	2.197	2.213	2.217	2.242
C ($J K^{-1} mol^{-1}$)	463.5	466.6	470.0	470.9	476.2

Name: 2,2,4,4,6,8,8–Heptamethylnonane
Formula: $C_{16}H_{34}$

CAS–RN: 4390–04–9
Group No.: 11–054
Molar Mass: 226.45

TABLE 11.54.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88COS/VAN	298.15	2.026	nosp	99.	anal	C_p	FSIT	71PIC/LED

Name: Hexadecane
Formula: $C_{16}H_{34}$

CAS–RN: 544–76–3
Group No.: 11–055
Molar Mass: 226.45

TABLE 11.55.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49PAR/MOO		290.0–300.0	2S	1.00	95.	estim	C_p	BSIO	25PAR
54FIN/GRO2	N	295.4–320.3	9	0.20	99.88	melpt	C_{sat}	BSAO	43RUE/HUF
56SCH/GOT		292.1–294.6	4	2.00	not specified		C_p	BSAO	33SOU/BRI
62GOL/BEL		310.9–422.0	3	nosp	96.9	chrom	C_p	BDHT	63GUD/CAM
68REC1	N	298.0–313.0	eqn	nosp	not specified		C_p	BSAO	68REC1
70AKH		293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS
71REC/SAD		303.1	1	0.30	not specified		C_p	BSIO	70REC
72REC/SAD		298.1	1	0.30	not specified		C_p	BSIO	70REC
73KAL/WOY		303.1	1	0.20	99.5	chrom	C_p	BSIO	70REC
74DIA/REN		300.1–323.5	9	0.30	not specified		C_p	BSAO	74DIA/REN
74PET/TER		297.8–453.5	14	1.00	98.	melpt	C_p	BDCT	74PET/TER
81GRO/ING		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
85COS/PAT5		298.2	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
86WIL/LAI		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
88COS/VAN		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
91BAN/GAR		318.1–373.1	12	0.40	99.4	chrom	C_p	BDCT	91BAN/GAR
91TRE/COS		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
92LAI/ROD		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

54FIN/GRO2 smoothed data in 67MES/GUT
68REC1 same data in 68REC3

TABLE 11.55.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO2	295.4–320.3	9	0.20	0.320	3.93–2	0.06	6.54–3	–1
73KAL/WOY	303.1	1	0.20	0.361	4.38–2	0.07	4.38–2	1
74DIA/REN	300.1–323.5	9	0.30	0.599	1.11–1	0.18	2.45–2	5
74PET/TER	297.8–395.8	11	1.00	0.853	5.35–1	0.85	–1.07–1	–5
88COS/VAN	298.1	1	0.50#	0.555	1.67–1	0.28	–1.67–1	–1
91BAN/GAR	318.1–373.1	12	0.40	0.265	6.81–2	0.11	–4.00–2	–8

Rejected data			
49PAR/MOO	(2.94–1, 0.48, 2.94–1, 1)	62GOL/BEL	(2.42, 4.05, –2.38, –2)
68REC1	(2.09–1, 0.34, –1.97–1, –4)	71REC/SAD	(6.87–1, 1.15, –6.87–1, –1)
72REC/SAD	(6.01–1, 1.01, –6.01–1, –1)	81GRO/ING	(1.96–1, 0.33, –1.96–1, –1)
85COS/PAT5	(2.41–1, 0.40, –2.41–1, –1)	86WIL/LAI	(7.06–1, 1.18, –7.06–1, –1)
89LAI/ROD	(5.34–1, 0.89, –5.34–1, –1)	91TRE/COS	(2.26–1, 0.38, –2.26–1, –1)
92LAI/ROD	(6.56–1, 1.10, –6.56–1, –1)		

TABLE 11.55.3. Parameters of regression polynomial

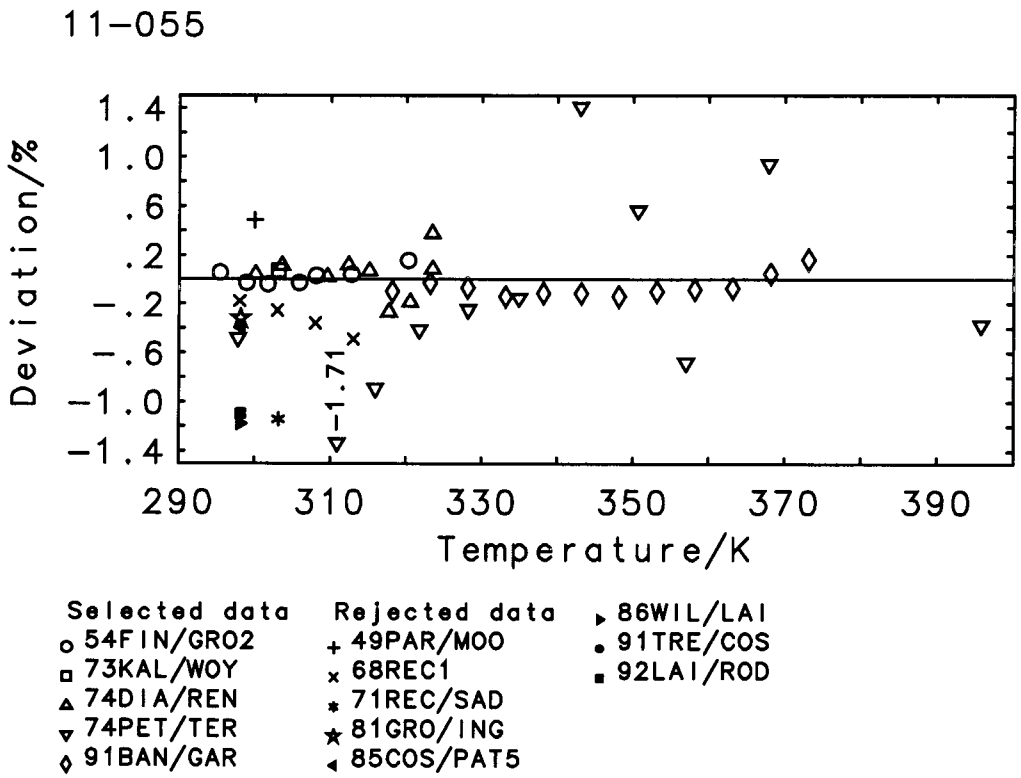
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	68	43	0.587	2.94–1	0.47	–3.49–2	–9
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
295.4–395.8		1.12967+2	–5.42802+1	1.65941+1	–1.44561		IV

TABLE 11.55.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	2.219	2.244	2.270	2.299	2.329	2.360	2.393
C ($J K^{-1} mol^{-1}$)	502.5	508.0	514.0	520.5	527.3	534.5	541.9
Temp. (K)	370	380	390	400			
c ($J K^{-1} g^{-1}$)	2.426	2.460	2.494	2.527			
C ($J K^{-1} mol^{-1}$)	549.4	557.1	564.7	572.3			

TABLE 11.55.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	68	43	0.655	2.94–1	0.47	–2.01–2	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
295.4–395.8	722.00	–1.32513+1	8.18227	3.70095+1	5.36517		IV



Name: Heptadecane
Formula: $C_{17}H_{36}$

CAS-RN: 629-78-7
Group No.: 11-056
Molar Mass: 240.47

TABLE 11.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67MES/GUT	301.9–384.4	11	0.20	99.89	melpt	C_{sat}	BSAO	47HUF
70AKH	293.1	1	nosp	not specified		C_p	BDHO	59ABA/MUS

TABLE 11.56.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
67MES/GUT	301.9–384.4	11	0.20#	0.305	4.07–2	0.06	4.51–5	1

TABLE 11.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	12	11	0.357	4.78–2	0.07	4.51–5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
301.9–384.4	5.77157+1	–3.13378	1.76927	II

TABLE 11.56.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_{sat} ($J K^{-1} g^{-1}$)	2.221	2.248	2.275	2.304	2.334	2.366	2.398
C_{sat} ($J K^{-1} mol^{-1}$)	534.1	540.5	547.1	554.1	561.3	568.9	576.7

Temp. (K)	370	380
c_{sat} ($J K^{-1} g^{-1}$)	2.432	2.467
C_{sat} ($J K^{-1} mol^{-1}$)	584.9	593.3

Name: Octadecane
Formula: $C_{18}H_{38}$

CAS-RN: 593-45-3
Group No.: 11-057
Molar Mass: 254.50

TABLE 11.57.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49PAR/MOO	300.0	1	1.00	96.	estim	C_p	BSIO	25PAR
67MES/GUT	304.4–378.7	11	0.20	99.98	melpt	C_{sat}	BSAO	47HUF
81HOE	325.0–375.0	3S	5.00	not specified		C_p	BDHT	69PER/COM
93DUR/AOU	373.0–473.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
49PAR/MOO	300.0	1	1.00	0.140	9.51–2	0.14	–9.51–2	–1
67MES/GUT	304.4–378.7	11	0.20#	0.378	5.29–2	0.08	–1.35–2	–4
93DUR/AOU	373.0–473.0	51	3.00#	0.628	1.50	1.88	7.31–1	19
				Rejected data				
81HOE	(2.38, 3.42, –2.36, –3)							

TABLE 11.57.3. Parameters of regression polynomial

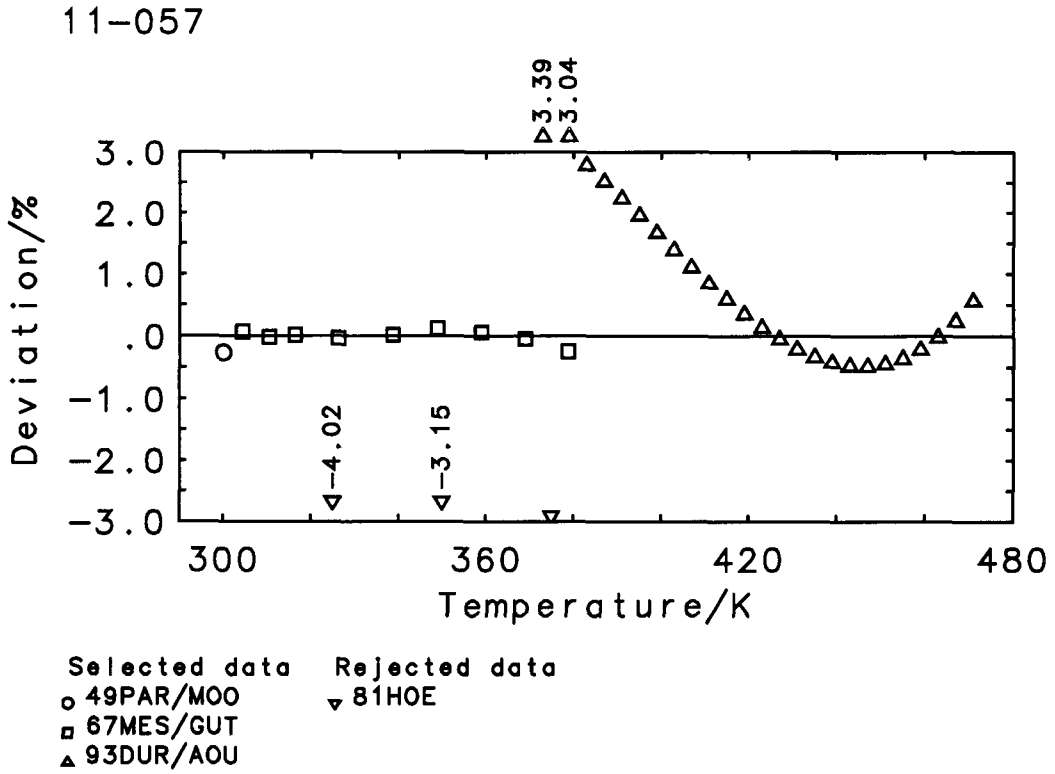
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	66	63	0.601	1.38	1.74	5.88–1	14
Temp. range K		A_1	A_2	A_3			Level of uncertainty
300.0–473.0		5.77808+1	–1.26076	1.55254			V

TABLE 11.57.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	2.221	2.247	2.275	2.304	2.334	2.365	2.397
C ($J K^{-1} mol^{-1}$)	565.1	572.0	579.1	586.4	594.0	601.9	610.0
Temp. (K)	370	380	390	400	410	420	430
c ($J K^{-1} g^{-1}$)	2.430	2.464	2.499	2.534	2.571	2.609	2.648
C ($J K^{-1} mol^{-1}$)	618.4	627.0	635.9	645.0	654.4	664.1	674.0
Temp. (K)	440	450	460	470			
c ($J K^{-1} g^{-1}$)	2.688	2.729	2.771	2.815			
C ($J K^{-1} mol^{-1}$)	684.2	694.6	705.3	716.3			

TABLE 11.57.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	66	63	1.375	1.32	1.62	–2.16–1	–7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
300.0–473.0	746.00	–1.66944+1	1.59290	3.87559+1	4.37413+1		V



Name: Nonadecane
Formula: $C_{19}H_{40}$

CAS-RN: 629-92-5
Group No.: 11-058
Molar Mass: 268.53

TABLE 11.58.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69ATK/LAR	305.0–453.0	eqn	nosp	99.9	chrom	C_p	BSAO	58WES/GIN
84GRI/AND	313.1–433.2	10	0.70	not specified		C_p	BSAO	67RAS/GAN
93DUR/AOU	373.0–473.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.58.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69ATK/LAR	305.0–453.0	9	0.50#	0.251	1.01–1	0.13	1.00–1	9
84GRI/AND	313.1–433.2	10	0.70	0.484	2.67–1	0.34	–1.74–1	–4
				Rejected data				
93DUR/AOU	(1.88, 2.25, 6.01–1, 8)							

TABLE 11.58.3. Parameters of regression polynomial

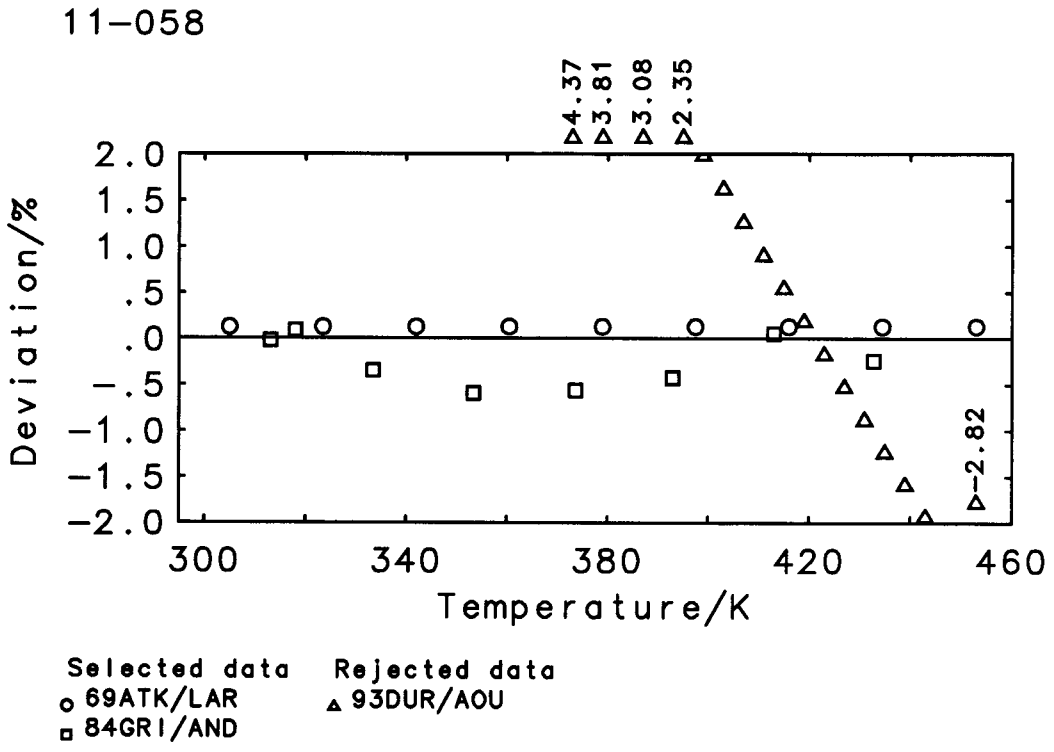
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	70	19	0.414	2.17–1	0.28	–4.42–2	5
Temp. range K		A_1	A_2				Level of uncertainty
305.0–453.0		3.83583+1	1.08986+1				IV

TABLE 11.58.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	2.234	2.268	2.301	2.335	2.369	2.403	2.436
C_p ($J K^{-1} mol^{-1}$)	599.8	608.9	618.0	627.0	636.1	645.1	654.2
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.470	2.504	2.538	2.571	2.605	2.639	2.673
C_p ($J K^{-1} mol^{-1}$)	663.3	672.3	681.4	690.5	699.5	708.6	717.6
Temp. (K)	450						
c_p ($J K^{-1} g^{-1}$)	2.706						
C_p ($J K^{-1} mol^{-1}$)	726.7						

TABLE 11.58.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	70	19	0.435	2.11–1	0.26	4.93–3	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
305.0–453.0	756.20	–1.01421+1	4.26039–1	4.13677+1	6.03592+1		IV



Name: 2,6,10,14–Tetramethylpentadecane
Formula: $C_{19}H_{40}$

CAS–RN: 1921–70–6
Group No.: 11–059
Molar Mass: 268.53

TABLE 11.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
93DUR/AOU	304.0–404.0	51	nosp	not	specified	C_p	BDCT	86MER/BEN

TABLE 11.59.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
91TRE/COS	298.1	1	0.50#	0.417	1.43–1	0.21	–1.43–1	–1
93DUR/AOU	304.0–404.0	51	5.00#	0.187	6.83–1	0.93	2.92–1	14

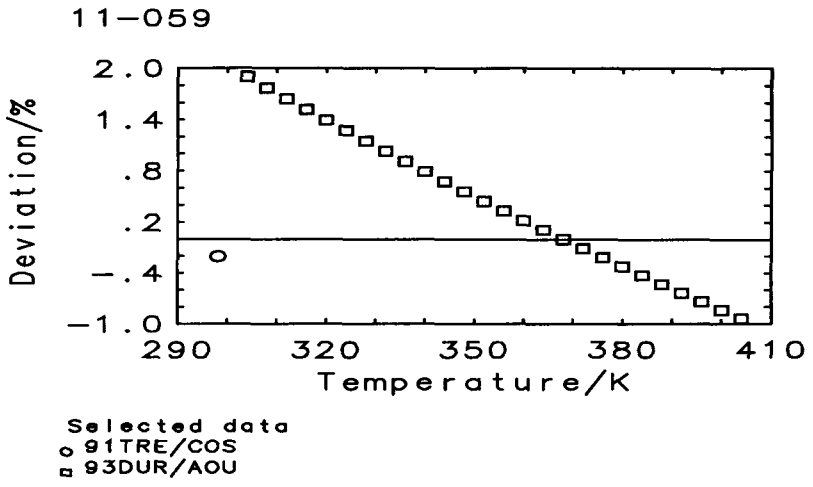
TABLE 11.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	52	52	0.198	6.90–1	0.94	2.84–1	13

Temp. range K	A_1	A_2	Level of uncertainty
298.1–404.0	3.43208+1	1.15204+1	VI

TABLE 11.59.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.13	2.17	2.20	2.24	2.28	2.31	2.35
C_p (J K^{-1}mol^{-1})	573	582	592	601	611	621	630
Temp. (K)	370	380	390	400			
c_p (J K^{-1}g^{-1})	2.38	2.42	2.45	2.49			
C_p (J K^{-1}mol^{-1})	640	649	659	669			



Name: Eicosane
Formula: $C_{20}H_{42}$

CAS-RN: 112-95-8
Group No.: 11-060
Molar Mass: 282.55

TABLE 11.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81HOE	325.0–400.0	4S	5.00	not specified		C_p	BDHT	69PER/COM

TABLE 11.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.143	6.05–1	0.71	5.18–3	0
Temp. range K		A_1	A_2				Level of uncertainty
325.0–400.0		2.89612+1	1.52350+1				VI

TABLE 11.60.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1}g^{-1}$)	2.29	2.33	2.38	2.42	2.47	2.51	2.56
C_p ($J K^{-1}mol^{-1}$)	646	659	671	684	697	709	722
Temp. (K)	390	400					
c_p ($J K^{-1}g^{-1}$)	2.60	2.65					
C_p ($J K^{-1}mol^{-1}$)	735	747					

Name: Heneicosane
Formula: $C_{21}H_{44}$

CAS-RN: 629-94-7
Group No.: 11-061
Molar Mass: 296.58

TABLE 11.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48MAZ	318.1–328.1	2	nosp	not specified		C_p	BDHO	33STR/MAL
84GRI/AND	315.9–433.1	8	0.80	not specified		C_p	BSAO	67RAS/GAN

TABLE 11.61.2. Correlated heat capacities

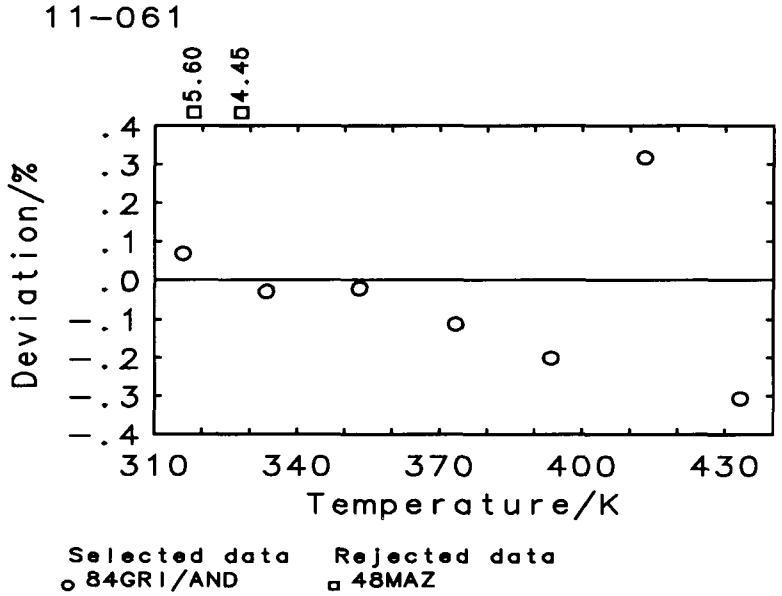
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
84GRI/AND	315.9–433.1	8	0.80	0.260	1.90–1	0.21	7.71–4	–2
				Rejected data				
48MAZ	(4.30, 5.05, 4.27, 2)							

TABLE 11.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	8	0.329	2.40–1	0.26	7.71–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
315.9–433.1		6.54526+1	–2.32741–1	1.54098			IV

TABLE 11.61.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.256	2.284	2.312	2.341	2.371	2.402	2.434
C_p (J K^{-1}mol^{-1})	669.2	677.3	685.7	694.4	703.3	712.4	721.9
Temp. (K)	390	400	410	420	430		
c_p (J K^{-1}g^{-1})	2.467	2.500	2.534	2.570	2.606		
C_p (J K^{-1}mol^{-1})	731.5	741.5	751.7	762.1	772.8		



Name: Docosane
Formula: $C_{22}H_{46}$

CAS-RN: 629–97–0
Group No.: 11–062
Molar Mass: 310.61

TABLE 11.62.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31GAR/VAN	317.5	1	nosp	not specified		C_p	DSIO	24GAR/RAN
69ATK/LAR	318.0–453.0	eqn	nosp	99.7	chrom	C_p	BSAO	58WES/GIN
81HOE	325.0–500.0	8S	5.00	not specified		C_p	BDHT	69PER/COM
93DUR/AOU	373.0–473.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.62.2. Correlated heat capacities

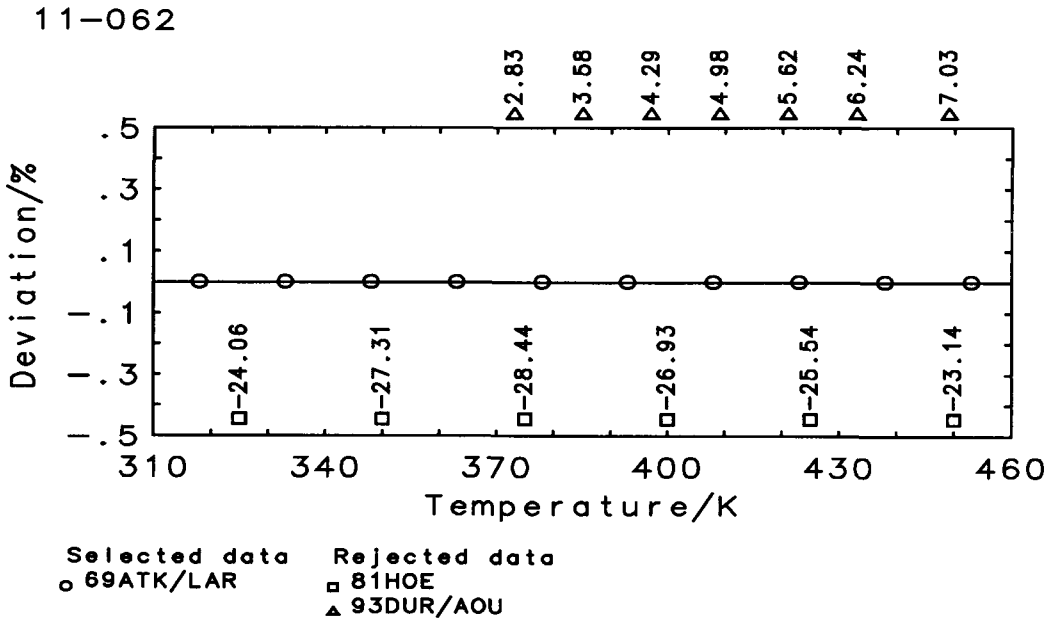
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69ATK/LAR	318.0–453.0	10	0.50#	0.000	4.18–6	0.00	–7.63–7	0
				Rejected data				
81HOE	(1.92+1, 25.97, –1.91+1, –6)			93DUR/AOU	(5.50, 5.29, 5.28, 41)			

TABLE 11.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	70	10	0.000	4.67–6	0.00	–7.63–7	0
Temp. range K		A_1	A_2				Level of uncertainty
318.0–453.0		4.38783+1	1.27388+1				V

TABLE 11.62.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.27	2.30	2.33	2.37	2.40	2.44	2.47
C_p (J K^{-1}mol^{-1})	704	714	725	736	746	757	767
Temp. (K)	390	400	410	420	430	440	450
c_p (J K^{-1}g^{-1})	2.50	2.54	2.57	2.61	2.64	2.67	2.71
C_p (J K^{-1}mol^{-1})	778	788	799	810	820	831	841



Name: Tricosane
Formula: $C_{23}H_{48}$

CAS-RN: 638-67-5
Group No.: 11-063
Molar Mass: 324.63

TABLE 11.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69ATK/LAR	321.0–453.0	eqn	nosp	99.9	chrom	C_p	BSAO	58WES/GIN

TABLE 11.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.000	5.39–6	0.00	3.05–6	0
Temp. range K		A_1	A_2				Level of uncertainty
321.0–453.3		4.44029+1	1.37045+1				V

TABLE 11.63.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1} g^{-1}$)	2.26	2.30	2.33	2.37	2.40	2.44	2.47
C_p ($J K^{-1} mol^{-1}$)	734	745	757	768	779	791	802
Temp. (K)	390	400	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	2.51	2.54	2.58	2.61	2.65	2.68	2.72
C_p ($J K^{-1} mol^{-1}$)	814	825	836	848	859	871	882

Name: Tetracosane
Formula: $C_{24}H_{50}$

CAS-RN: 646-31-1
Group No.: 11-064
Molar Mass: 338.66

TABLE 11.64.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48MAZ	325.1–334.1	2	nosp	not specified		C_p	BDHO	33STR/MAL
69ATK/LAR	324.0–453.0	eqn	nosp	99.9	chrom	C_p	BSAO	58WES/GIN
81HOE	350.0–425.0	4S	5.00	not specified		C_p	BDHT	69PER/COM
84GRI/AND	330.6–433.4	8	0.80	not specified		C_p	BSAO	67RAS/GAN

TABLE 11.64.2. Correlated heat capacities

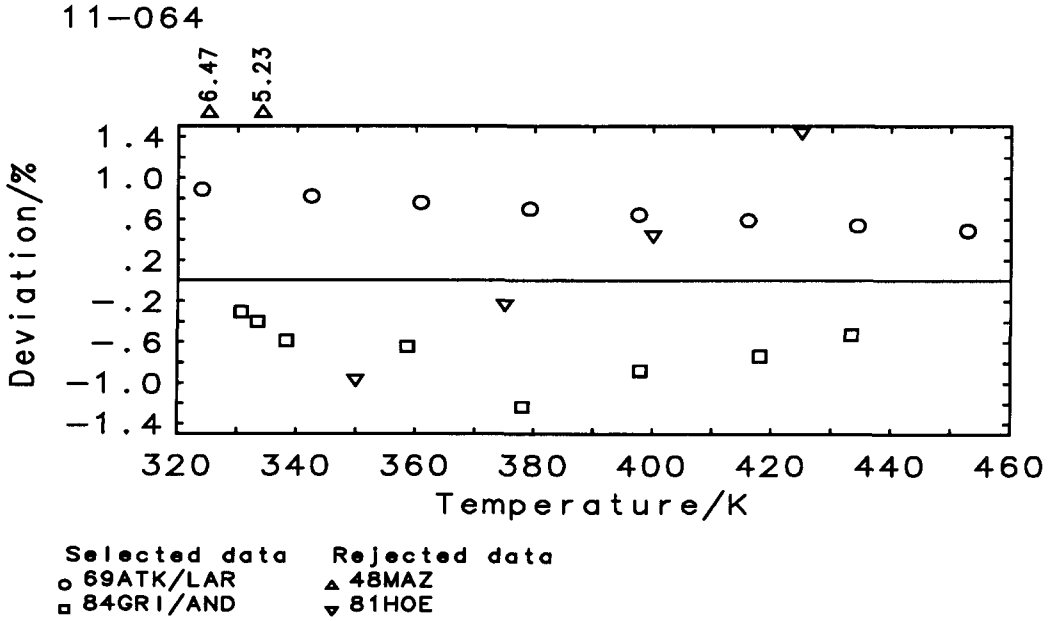
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
69ATK/LAR	324.0–452.8	8	0.80#	0.861	6.87–1	0.69	6.81–1	8
84GRI/AND	330.6–433.4	8	0.80	0.900	7.16–1	0.72	–6.60–1	–8
				Rejected data				
48MAZ	(5.81, 5.88, 5.78, 2)		81HOE	(9.38–1, 0.90, 2.17–1, 0)				

TABLE 11.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	22	16	0.942	7.50–1	0.75	1.03–2	0
Temp. range K		A_1	A_2				Level of uncertainty
324.0–452.8		4.84202+1	1.35427+1				IV

TABLE 11.64.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	2.286	2.319	2.352	2.386	2.419	2.452	2.485
C_p ($J K^{-1} mol^{-1}$)	774.2	785.4	796.7	808.0	819.2	830.5	841.7
Temp. (K)	400	410	420	430	440	450	
c_p ($J K^{-1} g^{-1}$)	2.519	2.552	2.585	2.618	2.652	2.685	
C_p ($J K^{-1} mol^{-1}$)	853.0	864.3	875.5	886.8	898.0	909.3	



Name: Pentacosane
Formula: $C_{25}H_{52}$

CAS–RN: 629–99–2
Group No.: 11–065
Molar Mass: 352.69

TABLE 11.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
32SPA/THO	333.1–373.1	5S	1.00	not specified		C_p	BDHO	31THO/PAR

TABLE 11.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.056	5.61–2	0.06	4.42–5	0
Temp. range K		A_1	A_2				Level of uncertainty
333.1–373.1		4.90533+1	1.47254+1				V

TABLE 11.65.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	2.30	2.34	2.37	2.41	2.44
C_p ($J K^{-1} mol^{-1}$)	812	824	836	849	861

Name: Hexacosane
Formula: $C_{26}H_{54}$

CAS–RN: 630–01–3
Group No.: 11–066
Molar Mass: 366.71

TABLE 11.66.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31GAR/VAN	329.3	1	nosp	not specified		C_p	DSIO	24GAR/RAN
69ATK/LAR	329.0–453.0	eqn	nosp	99.8	chrom	C_p	BSAO	58WES/GIN
76AND/MAR	332.2–358.6	10	0.10	99.77	melpt	C_p	BSAO	68WES/FUR

TABLE 11.66.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69ATK/LAR	329.0–453.6	15	0.80#	0.523	4.34–1	0.42	–1.24–1	0
76AND/MAR	332.2–358.6	10	0.10	0.295	3.06–2	0.03	3.02–3	4
				Rejected data				
31GAR/VAN	(1.38, 1.33, 1.38, 1)							

TABLE 11.66.3. Parameters of regression polynomial

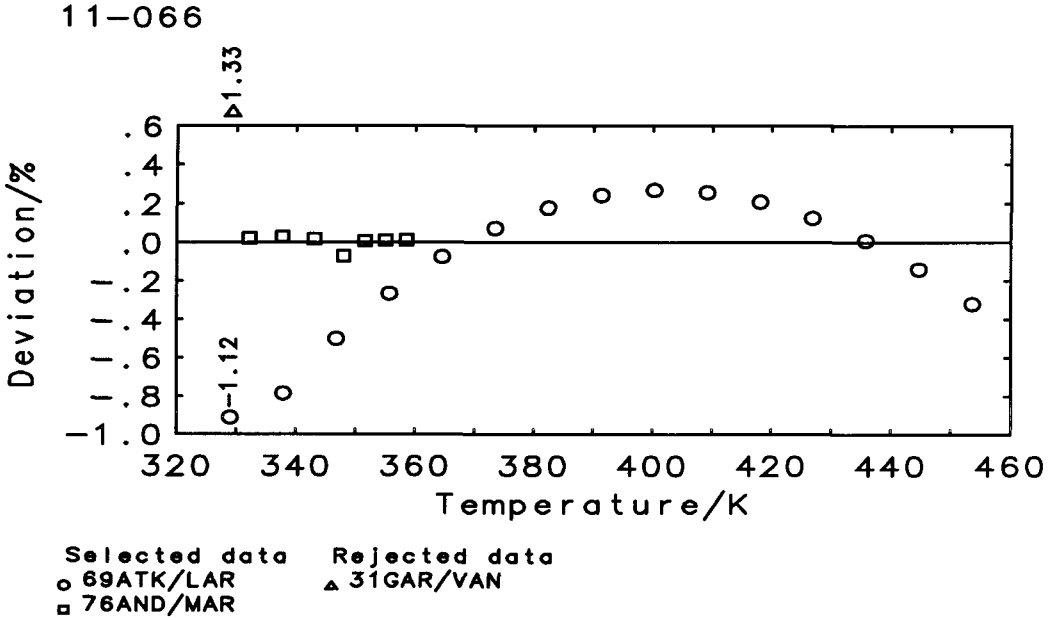
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	25	0.475	3.59–1	0.35	–7.35–2	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
329.0–453.6		9.12413+1	–5.44480	2.64279			III

TABLE 11.66.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p (J K^{-1}g^{-1})	2.314	2.342	2.371	2.401	2.432	2.465	2.499
C_p (J K^{-1}mol^{-1})	848.5	858.7	869.4	880.4	891.9	903.9	916.3
Temp. (K)	400	410	420	430	440	450	
c_p (J K^{-1}g^{-1})	2.534	2.570	2.607	2.646	2.686	2.727	
C_p (J K^{-1}mol^{-1})	929.1	942.4	956.1	970.3	984.8	999.9	

TABLE 11.66.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	24	3.255	3.47–1	0.34	1.47–1	8
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
329.0–452.5	817.00	–1.31216+1	4.26776–1	5.29851+1	1.00859+2		IV



Name: Heptacosane
Formula: $C_{27}H_{56}$

CAS–RN: 593–49–7
Group No.: 11–067
Molar Mass: 380.74

TABLE 11.67.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38VER	N	338.15	2.176	nosp	not specified		avg	BDHO	33STR/MAL

38VER average value in temperature range 332–342 K

Name: Octacosane
Formula: $C_{28}H_{58}$

CAS-RN: 630-02-4
Group No.: 11-068
Molar Mass: 394.77

TABLE 11.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53HOF/DEC	343.1–353.1	2	4.00	90.	estim	C_p	BDHO	52HOF
69ATK/LAR	334.0–453.0	eqn	nosp	99.9	chrom	C_p	BSAO	58WES/GIN
93DUR/AOU	373.0–473.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.68.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69ATK/LAR	334.0–452.8	13	0.80#	0.000	5.60–6	0.00	–4.11–6	0
				Rejected data				
53HOF/DEC	(1.70, 1.55, –1.69, –2)			93DUR/AOU	(1.71, 1.47, –1.42, –34)			

TABLE 11.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	66	13	0.000	6.09–6	0.00	–4.11–6	0
Temp. range K		A_1	A_2				Level of uncertainty
334.0–452.8		5.55775+1	1.61905+1				IV

TABLE 11.68.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1}g^{-1}$)	2.330	2.364	2.398	2.432	2.466	2.500	2.535
C_p ($J K^{-1}mol^{-1}$)	919.8	933.3	946.7	960.2	973.6	987.1	1001
Temp. (K)	410	420	430	440	450		
c_p ($J K^{-1}g^{-1}$)	2.569	2.603	2.637	2.671	2.705		
C_p ($J K^{-1}mol^{-1}$)	1014	1027	1041	1054	1068		

Name: 2,6,10,15,19,23-Hexamethyltetracosane
Formula: $C_{30}H_{62}$

CAS-RN: 111-01-3
Group No.: 11-069
Molar Mass: 422.82

TABLE 11.69.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
93DUR/AOU	304.0–404.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.69.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
91TRE/COS	298.1	1	0.50#	0.882	4.70–1	0.44	–4.70–1	–1
93DUR/AOU	304.0–404.0	51	3.00#	0.229	7.51–1	0.69	3.45–1	15

TABLE 11.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	52	52	0.262	7.61–1	0.70	3.29–1	14
Temp. range K		A_1	A_2				Level of uncertainty
298.1–404.0		9.25703+1	4.86460				V

TABLE 11.69.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.11	2.12	2.13	2.14	2.15	2.16	2.16
C_p (J K^{-1}mol^{-1})	891	895	899	903	907	911	915
Temp. (K)	370	380	390	400			
c_p (J K^{-1}g^{-1})	2.17	2.18	2.19	2.20			
C_p (J K^{-1}mol^{-1})	919	923	927	931			

Name: Triacontane
Formula: $C_{30}H_{62}$

CAS–RN: 638–68–6
Group No.: 11–070
Molar Mass: 422.82

TABLE 11.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31GAR/VAN	338.5	1	nosp	not specified		C_p	DSIO	24GAR/RAN
48MAZ	340.1–350.1	2	nosp	not specified		C_p	BDHO	33STR/MAL
81HOE	350.0–450.0	5S	5.00	not specified		C_p	BDHT	69PER/COM
93DUR/AOU	373.0–473.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.70.2. Correlated heat capacities

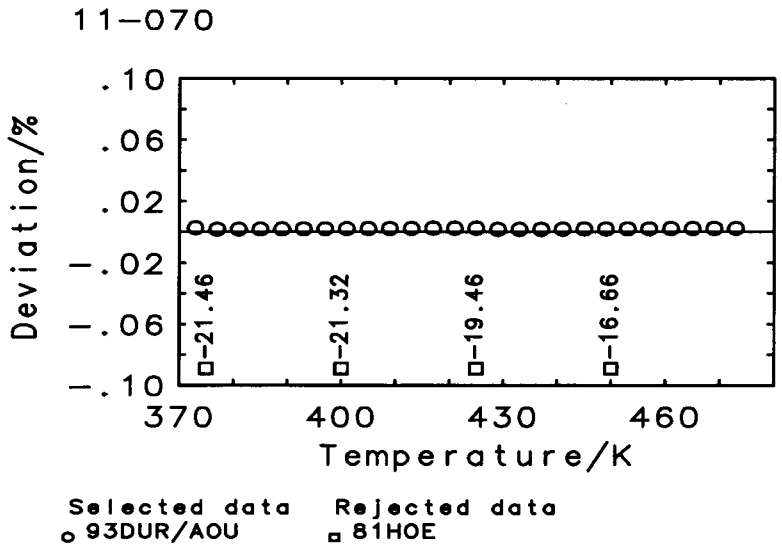
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
93DUR/AOU	373.0–473.0	51	3.00#	0.000	3.32–4	0.00	2.99–6	0
				Rejected data				
81HOE	(2.08+1, 19.82, –2.07+1, –4)							

TABLE 11.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	59	51	0.000	3.39–4	0.00	2.99–6	0
Temp. range K		A_1	A_2				Level of uncertainty
373.0–473.0		7.74907+1	1.17846+1				VI

TABLE 11.70.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.38	2.40	2.43	2.45	2.47	2.50	2.52
C_p (J K^{-1}mol^{-1})	1010	1020	1030	1040	1050	1060	1070
Temp. (K)	440	450	460	470			
c_p (J K^{-1}g^{-1})	2.54	2.57	2.59	2.61			
C_p (J K^{-1}mol^{-1})	1080	1090	1100	1100			



Name: 11–Decylheneicosane
Formula: $C_{31}H_{64}$

CAS–RN: 55320–06–4
Group No.: 11–071
Molar Mass: 436.85

TABLE 11.71.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
45FIS/NAY	N	282.0–297.4	5	0.70	96.6	melpt	C_p	BSIO	25PAR
45FIS/NAY	N	283.8–297.8	23	0.20	96.48	melpt	C_p	BSAO	47AST/SZA

45FIS/NAY the same sample measured at Stanford University, Stanford, CA
45FIS/NAY the same sample measured at Pennsylvania State University, University Park, PA

TABLE 11.71.2. Correlated heat capacities

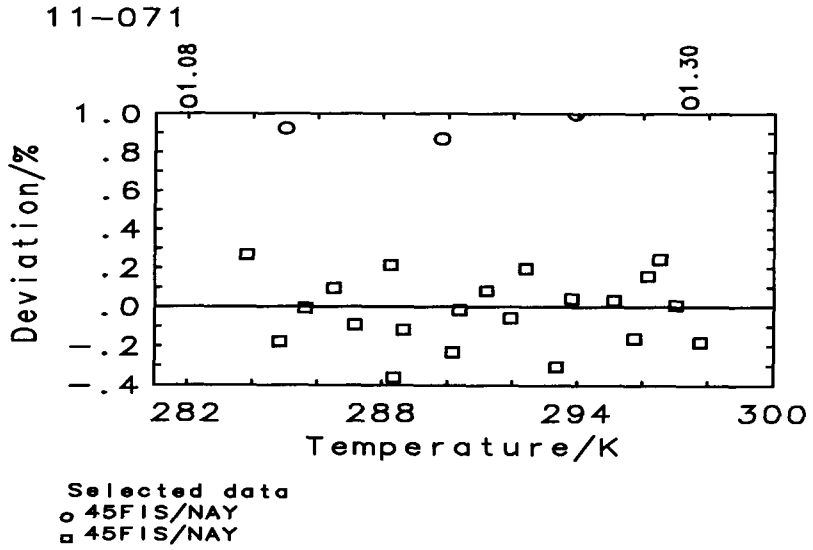
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
45FIS/NAY	282.0–297.4	5	0.70	1.489	1.19	1.04	1.18	5
45FIS/NAY	283.8–297.8	23	0.20	0.851	1.92–1	0.17	–1.98–2	–1

TABLE 11.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	28	1.033	5.52–1	0.48	1.94–1	4
Temp. range K		A_1	A_2				Level of uncertainty
282.0–297.8		6.68867+1	1.58226+1				III

TABLE 11.71.4. Recommended values of heat capacities

Temp. (K)	290	295	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.146	2.161	2.171	2.176
C_p ($J\,K^{-1}mol^{-1}$)	937.6	944.2	948.4	950.8



Name: Hentriacontane
Formula: $C_{31}H_{64}$

CAS-RN: 630–04–6
Group No.: 11–072
Molar Mass: 436.85

TABLE 11.72.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38VER	N	346.65	2.510	nosp	not specified		avg	BDHO	33STR/MAL

38VER average value in temperature range 341–351 K

Name: Dotriacontane
Formula: $C_{32}H_{66}$

CAS–RN: 544–85–4
Group No.: 11–073
Molar Mass: 450.88

TABLE 11.73.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38VER	N	348.1	1	nosp	not specified		avg	BDHO	33STR/MAL
81HOE		350.0–475.0	6S	5.00	not specified		C_p	BDHT	69PER/COM

38VER average value in temperature range 343–353 K

TABLE 11.73.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
81HOE	350.0–475.0	6	5.00	0.195	1.23	0.98	2.57–2	2

TABLE 11.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.239	1.51	1.20	2.57–2	2

Temp. range K	A_1	A_2	Level of uncertainty
350.0–475.0	7.27042+1	1.30208+1	VI

TABLE 11.73.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1} g^{-1}$)	2.18	2.21	2.23	2.25	2.28	2.30	2.33
C_p ($J K^{-1} mol^{-1}$)	983	994	1010	1020	1030	1040	1050
Temp. (K)	420	430	440	450	460	470	480
c_p ($J K^{-1} g^{-1}$)	2.35	2.37	2.40	2.42	2.45	2.47	2.49
C_p ($J K^{-1} mol^{-1}$)	1060	1070	1080	1090	1100	1110	1120

Name: Tritriacontane
Formula: $C_{33}H_{68}$

CAS–RN: 630–05–7
Group No.: 11–074
Molar Mass: 464.90

TABLE 11.74.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
32SPA/THO	353.1–383.1	4S	1.00	not specified		C_p	BDHO	31THO/PAR

TABLE 11.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	4	0.066	9.06–2	0.07	4.96–5	0
Temp. range K		A_1	A_2				Level of uncertainty
353.1–383.1		7.84717+1	1.56849+1				V

TABLE 11.74.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380
c_p ($J K^{-1}g^{-1}$)	2.39	2.41	2.44	2.47
C_p ($J K^{-1}mol^{-1}$)	1110	1120	1130	1150

Name: Tetratriacontane
Formula: $C_{34}H_{70}$

CAS-RN: 14167–59–0
Group No.: 11–075
Molar Mass: 478.93

TABLE 11.75.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31GAR/VAN	346.3	1	nosp	not specified		C_p	DSIO	24GAR/RAN
69ATK/LAR	346.0–453.0	eqn	nosp	99.8	chrom	C_p	BSAO	58WES/GIN

TABLE 11.75.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
69ATK/LAR	346.0–452.7	12	0.50#	0.000	7.63–6	0.00	–3.82–6	0
				Rejected data				
31GAR/VAN	(4.80–1, 0.35, 4.80–1, 1)							

TABLE 11.75.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	13	12	0.000	8.36–6	0.00	–3.82–6	0
Temp. range K		A_1	A_2				Level of uncertainty
346.0–452.7		6.80640+1	1.98726+1				IV

TABLE 11.75.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.389	2.424	2.458	2.493	2.527	2.562	2.596
C_p (J K^{-1}mol^{-1})	1144	1161	1177	1194	1210	1227	1243
Temp. (K)	420	430	440	450			
c_p (J K^{-1}g^{-1})	2.631	2.665	2.700	2.734			
C_p (J K^{-1}mol^{-1})	1260	1276	1293	1309			

Name: Pentatriacontane
Formula: $C_{35}H_{72}$

CAS-RN: 630-07-9
Group No.: 11-076
Molar Mass: 492.96

TABLE 11.76.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
31GAR/VAN	347.15	2.368	nosp	not specified	C_p	DSIO	24GAR/RAN

Name: Hexatriacontane
Formula: $C_{36}H_{74}$

CAS-RN: 630-06-8
Group No.: 11-077
Molar Mass: 506.98

TABLE 11.77.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
48MAZ	350.1-359.1	2	nosp	not specified	C_p	BDHO	33STR/MAL
69ATK/LAR	349.0-453.0	eqn	nosp	not specified	C_p	BSAO	58WES/GIN
81HOE	375.0-500.0	6S	5.00	not specified	C_p	BDHT	69PER/COM
91JIN/WUN	360.0-430.0	8	1.00	98. anal	C_p	BDHT	90JIN/WUN
93DUR/AOU	373.0-473.0	51	nosp	not specified	C_p	BDCT	86MER/BEN

TABLE 11.77.2. Correlated heat capacities

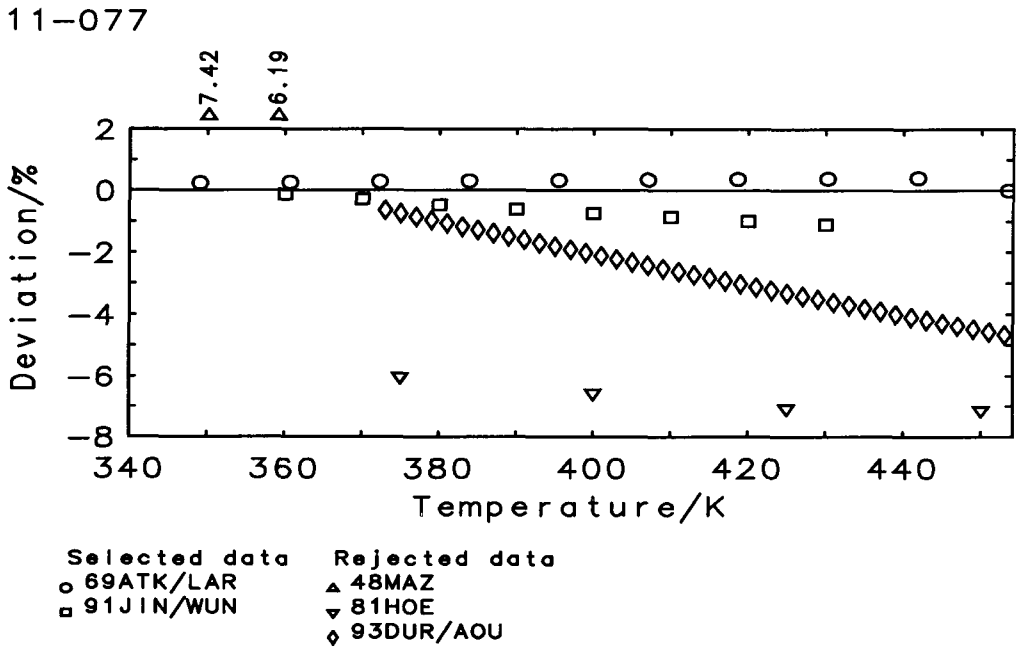
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
69ATK/LAR	349.0-453.4	10	0.80#	0.428	5.42-1	0.34	5.29-1	10
91JIN/WUN	360.0-430.0	8	1.00	0.725	1.13	0.73	-1.01	-8
				Rejected data				
48MAZ	(1.06+1, 6.83, 1.06+1, 2)			81HOE	(9.95, 6.72, -9.91, -4)			
93DUR/AOU	(4.59, 2.95, -4.17, -41)							

TABLE 11.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	77	18	0.615	9.07–1	0.58	–1.54–1	2
Temp. range K		A_1	A_2				Level of uncertainty
349.0–453.4		6.97449+1	2.12293+1				IV

TABLE 11.77.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.362	2.397	2.432	2.467	2.502	2.536	2.571
C_p (J K^{-1}mol^{-1})	1198	1215	1233	1251	1268	1286	1304
Temp. (K)	420	430	440	450			
c_p (J K^{-1}g^{-1})	2.606	2.641	2.676	2.711			
C_p (J K^{-1}mol^{-1})	1321	1339	1357	1374			



Name: Tetracontane
Formula: $C_{40}H_{82}$

CAS–RN: 4181–95–7
Group No.: 11–078
Molar Mass: 563.09

TABLE 11.78.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48MAZ	355.1–363.1	2	nosp	not specified		C_p	BDHO	33STR/MAL

TABLE 11.78.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
355.1–363.1		1.70014+2					VI

TABLE 11.78.4. Recommended values of heat capacities

Temp. (K)	355	365
c_p (J K^{-1}g^{-1})	2.51	2.51
C_p (J K^{-1}mol^{-1})	1410	1410

Name: Dotetracontane
Formula: $C_{42}H_{86}$

CAS–RN: 7098–20–6
Group No.: 11–079
Molar Mass: 591.14

TABLE 11.79.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69ATK/LAR	357.0–453.0	eqn	nosp	99.8	chrom	C_p	BSAO	58WES/GIN

TABLE 11.79.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	7.63–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
357.0–453.3		7.44141+1	2.74438+1				IV

TABLE 11.79.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c_p (J K^{-1}g^{-1})	2.436	2.475	2.513	2.552	2.591	2.629	2.668
C_p (J K^{-1}mol^{-1})	1440	1463	1486	1509	1531	1554	1577
Temp. (K)	430	440	450				
c_p (J K^{-1}g^{-1})	2.706	2.745	2.784				
C_p (J K^{-1}mol^{-1})	1600	1623	1646				

Name: Tritetracontane
Formula: $C_{43}H_{88}$

CAS–RN: 7098–21–7
Group No.: 11–080
Molar Mass: 605.17

TABLE 11.80.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48MAZ	359.1–364.1	2	nosp	not specified		C_p	BDHO	33STR/MAL

TABLE 11.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
359.1–364.1		1.91855+2					VI

TABLE 11.80.4. Recommended values of heat capacities

Temp. (K)	360
c_p (J K^{-1}g^{-1})	2.64
C_p (J K^{-1}mol^{-1})	1600

Name: Tetratetracontane
Formula: $C_{44}H_{90}$

CAS–RN: 7098–22–8
Group No.: 11–081
Molar Mass: 619.20

TABLE 11.81.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91JIN/WUN	370.0–430.0	7	1.00	99.	anal	C_p	BDHT	90JIN/WUN

TABLE 11.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.044	8.24–2	0.04	6.97–5	0
Temp. range K		A_1	A_2				Level of uncertainty
370.0–430.0		1.05179+2	2.08976+1				IV

TABLE 11.81.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.451	2.479	2.507	2.535	2.563	2.591	2.619
C_p (J K^{-1}mol^{-1})	1517	1535	1552	1570	1587	1604	1622

Name: Octatetracontane
Formula: $C_{48}H_{98}$

CAS–RN: 7098–26–2
Group No.: 11–082
Molar Mass: 675.31

TABLE 11.82.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
69ATK/LAR	363.0–453.0	eqn	nosp	95.	estim	C_p	BSAO	58WES/GIN

TABLE 11.82.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	9.34–6	0.00	4.58–6	0
Temp. range K		A_1	A_2				Level of uncertainty
363.0–453.0		9.63604+1	2.70463+1				IV

TABLE 11.82.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1}g^{-1}$)	2.419	2.452	2.485	2.518	2.552	2.585	2.618
C_p ($J K^{-1}mol^{-1}$)	1633	1656	1678	1701	1723	1746	1768
Temp. (K)	440	450					
c_p ($J K^{-1}g^{-1}$)	2.652	2.685					
C_p ($J K^{-1}mol^{-1}$)	1791	1813					

Name: Pentacontane
Formula: $C_{50}H_{102}$

CAS–RN: 6596–40–3
Group No.: 11–083
Molar Mass: 703.36

TABLE 11.83.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91JIN/WUN	380.0–430.0	6	1.00	99.	anal	C_p	BDHT	90JIN/WUN
93DUR/AOU	373.0–473.0	102	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 11.83.2. Correlated heat capacities

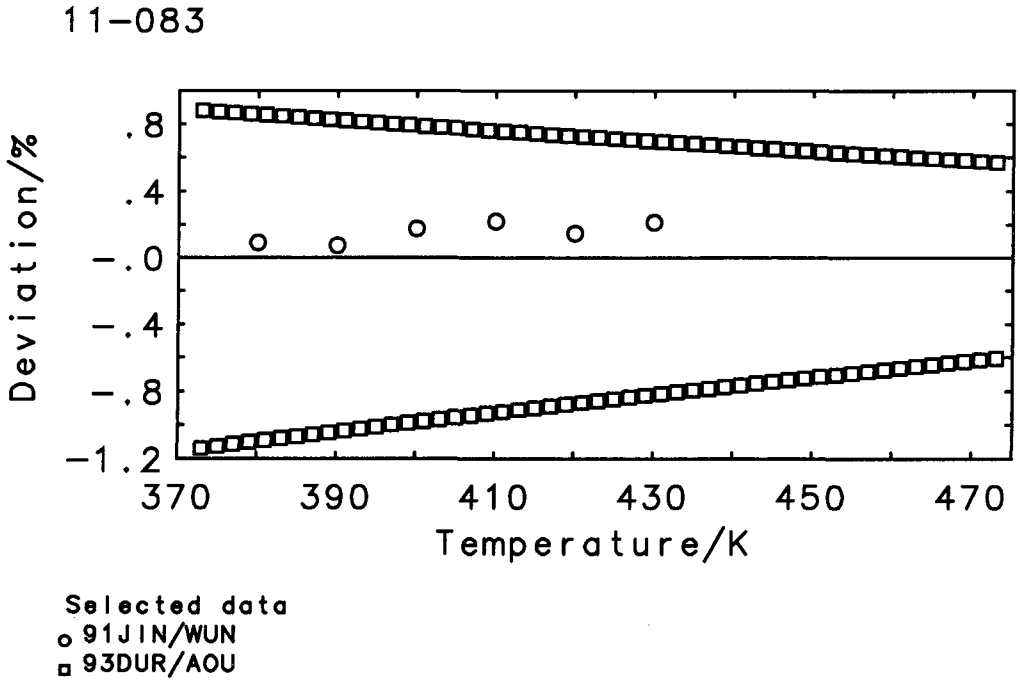
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
91JIN/WUN	380.0–430.0	6	1.00	0.161	3.50–1	0.16	3.27–1	6
93DUR/AOU	373.0–473.0	102	3.00#	0.269	1.74	0.81	–1.45–1	0

TABLE 11.83.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	108	108	0.266	1.71	0.79	–1.19–1	6
Temp. range K		A_1	A_2				Level of uncertainty
373.0–473.0		1.21050+2	2.31803+1				V

TABLE 11.83.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.445	2.472	2.500	2.527	2.554	2.582	2.609
C_p (J K^{-1}mol^{-1})	1720	1739	1758	1777	1797	1816	1835
Temp. (K)	440	450	460	470			
c_p (J K^{-1}g^{-1})	2.637	2.664	2.691	2.719			
C_p (J K^{-1}mol^{-1})	1855	1874	1893	1912			



12. Saturated Cyclic Hydrocarbons

This family contains data on 124 cyclic hydrocarbons; for 14 compounds data are available at a single temperature only. By definition, this family includes hydrocarbons without an unsaturated bond in the ring; however, an unsaturated bond may appear in a side chain.

Measurements for more than one half of the compounds were carried out at MRCE (62GOL/BEL, 63GUD/CAM) which was interested in this group of compounds because of their potential use as jet fuels. However, the purity of the samples was low and they were not sufficiently identified with respect to the specification of isomers and stereoisomers. For each compound, the heat capacity was usually measured at four temperatures in the range from 313 to 483 K using a differential heat conduction calorimeter developed by the authors; the data were obtained with the reported error of around 1 %, which we considered as realistic.

A great deal of effort was devoted to the measurement of the heat capacity of cycloalkanes and substituted cycloalkanes at BMB. Altogether, high-purity samples for 27 compounds were studied. The investigations gave results with a reported error of 0.2 %. All the experimental data (43RUE/HUF, 46DOU/HUF1, 49HUF/TOD, 50SCO/FIN2, 53GRO/OLI, 56FIN/SCO, 57MCC/FIN2, 65FIN/MES, 65MES/TOD1, 72FIN/MCC, 81FIN/MES) have been used as a basis for the final correlation of this monograph.

The data for the first two members of the homologous series, cyclopropane and cyclobutane, were measured only at UCB (46RUE/POW, 53RAT/GWI) using an isoperibol calorimeter (37GIA/EGA) where results showed a reported measurement error of 0.2 %.

Reliable data for cyclopentane were obtained at BMB (46DOU/HUF1). Data for the same compound were also measured at PSC (43AST/FIN) and repeatedly investigated by the same laboratory (47SZA/MOR). The authors of the former data reported an error of about 1 %, and, therefore, we have included only the values from the latter source in the final correlation.

The data on cyclohexane are the most abundant and this abundance corresponds to the importance of this compound to the chemical industry; however, data from different sources often differ by several percent. Altogether, 10 data sets containing heat capacity as a function of temperature have been selected for the final correlation. The data measured at BMB (43RUE/HUF) have been considered to be the most reliable source in the literature, unfortunately, measurements are available only over a narrow temperature interval (20 K). These values have been supplemented by the data obtained at GPI (78SAF) which were measured in two different calorimeters (a flow isoperibol calorimeter and an adiabatic calorimeter with continuous heating) and were mutually consistent. At the same time, these values agreed reasonably with the Bartlesville data (43RUE/HUF). Further, several additional data sets have been used in the correlation, such as: measurements from UGG (66KLE) in the temperature range from 293 to 343 K, high-temperature data up to 523 K from MITC (75SAN), and data from CITP (50AUE/SAG) with a reported error about 1.5 %. The data from the last mentioned laboratory (51CON/SAG) have been selected for the correlation of methylcyclopentane together with the BMB data (46DOU/HUF1).

The data on methylcyclohexane are the second most abundant in the family. We have selected three data sets which show excellent consistency and agreement: they are the BMB values (46DOU/HUF1), the direct experimental data from GITA (66HWA/ZIE) and later data available as a smoothing equation from the same laboratory (75HOL/ZIE).

Accurate data measured at the BMB (57MCC/FIN2) for two stereoisomers of the decahydronaphthalenes have been supplemented for the *trans* isomer by the less accurate data from the University of California at Los Angeles (53SEY) which were obtained by graphically smoothing the experimental values. The latter data have been included for extending the temperature range of recommendations. Seyer (53SEY) reported a sharp lambda peak around 323 K for *cis*-decahydronaphthalene. This anomaly was not confirmed by the accurate measurements at Bartlesville and for that reason the Seyer's data have not been not considered.

Bicyclic and condensed cycloalkanes were investigated primarily because of their interesting molecular structure. The main contributions originate from: UMAA (70WON/WES), MSUM (64SER/GOR) and KSUK (78SPI/AND).

Name: Cyclopropane
Formula: C_3H_6

CAS-RN: 75-19-4
Group No.: 12-001
Molar Mass: 42.08

TABLE 12.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
46RUE/POW	153.6–242.8	14	0.20	99.97	melpt	C_p	BSIO	28GIA/WIE1

TABLE 12.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	1.115	2.15–2	0.22	7.28–5	–2
C_{sat}	14	14	1.133	2.18–2	0.23	7.51–5	–2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
153.6–242.8	1.28210+1	–4.50403	1.34254	II
153.6–242.8	1.27017+1	–4.36964	1.30505	II

TABLE 12.1.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J K^{-1}g^{-1}$)	1.788	1.787	1.791	1.800	1.814	1.834	1.859
C_p ($J K^{-1}mol^{-1}$)	75.26	75.20	75.36	75.74	76.35	77.18	78.24
c_{sat} ($J K^{-1}g^{-1}$)	1.788	1.787	1.791	1.800	1.814	1.834	1.858
C_{sat} ($J K^{-1}mol^{-1}$)	75.26	75.20	75.37	75.75	76.35	77.16	78.20

Temp. (K)	230	240
c_p ($J K^{-1}g^{-1}$)	1.890	1.925
C_p ($J K^{-1}mol^{-1}$)	79.52	81.02
c_{sat} ($J K^{-1}g^{-1}$)	1.888	1.923
C_{sat} ($J K^{-1}mol^{-1}$)	79.45	80.91

TABLE 12.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	1.055	2.04–2	0.21	4.42–5	–3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
160.4–242.8	398.30	4.32889+2	4.04788+1	–4.66083+1	5.18080+2	–1.88430+2	5.03569+2	II

Name: Cyclobutane
Formula: C_4H_8

CAS-RN: 287-23-0
Group No.: 12-002
Molar Mass: 56.11

TABLE 12.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53RAT/GWI	184.8–284.6	19	0.20	99.81	melpt	C_p	BSIO	28GIA/WIE1

TABLE 12.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	1.626	3.90–2	0.33	2.06–4	5
C_{sat}	19	19	1.643	3.94–2	0.33	2.10–4	5

Temp. range K	A_1	A_2	A_3	Level of uncertainty
184.8–284.6	1.18155+1	–2.22040	8.95024–1	III
184.8–284.6	1.16660+1	–2.07935	8.62119–1	III

TABLE 12.2.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	1.605	1.623	1.645	1.669	1.696	1.725	1.757
C_p ($J\,K^{-1}mol^{-1}$)	90.03	91.08	92.29	93.64	95.15	96.80	98.60
c_{sat} ($J\,K^{-1}g^{-1}$)	1.605	1.624	1.645	1.669	1.696	1.725	1.757
C_{sat} ($J\,K^{-1}mol^{-1}$)	90.03	91.09	92.30	93.66	95.15	96.79	98.58

Temp. (K)	260	270	273.15	280	290	298.15
c_p ($J\,K^{-1}g^{-1}$)	1.792	1.829	1.842	1.869	1.912	1.949
C_p ($J\,K^{-1}mol^{-1}$)	100.5	102.6	103.3	104.9	107.3	109.3
c_{sat} ($J\,K^{-1}g^{-1}$)	1.791	1.828	1.840	1.868	1.910	1.946
C_{sat} ($J\,K^{-1}mol^{-1}$)	100.5	102.6	103.3	104.8	107.1	109.2

TABLE 12.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	1.820	4.35–2	0.36	2.63–4	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
184.8–284.6	460.00	–1.82709–1	2.01495	7.29198	4.14188–3	III

Name: Methylenecyclobutane
Formula: C_5H_8

CAS-RN: 1120–56–5
Group No.: 12–003
Molar Mass: 68.12

TABLE 12.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78LEB/TSV1	N	139.8–301.0	35	0.20	99.50	melpt	C_p	BSAO	76LEB/LIT
81FIN/MES		146.4–300.8	17	0.10	99.65	melpt	C_{sat}	BSAO	43RUE/HUF

78LEB/TSV1 same data in 78LEB/TSV2

TABLE 12.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
78LEB/TSV1	139.8–196.8	17	0.40#	0.238	1.24–2	0.10	3.27–3	2
81FIN/MES	146.4–300.8	17	0.20#	0.215	6.26–3	0.04	–8.05–4	–1

TABLE 12.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	52	34	0.241	1.05–2	0.08	1.23–3	1

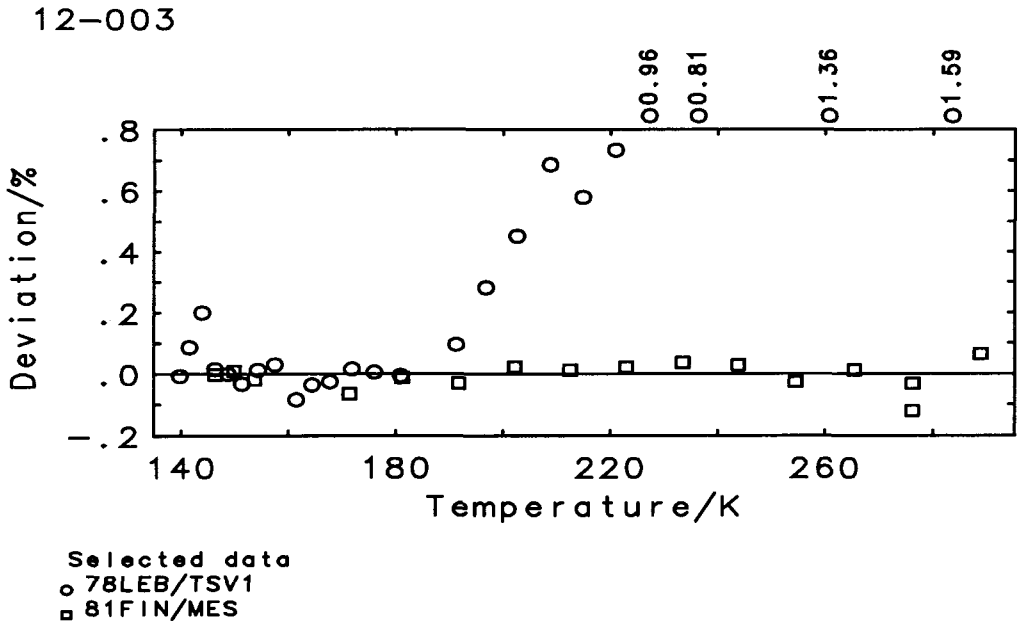
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
139.8–300.8	1.91024+1	–8.78714	3.60681	–3.47169–1	II

TABLE 12.3.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c ($J K^{-1} g^{-1}$)	1.577	1.570	1.569	1.572	1.580	1.592	1.609
C ($J K^{-1} mol^{-1}$)	107.4	107.0	106.9	107.1	107.6	108.5	109.6
Temp. (K)	210	220	230	240	250	260	270
c ($J K^{-1} g^{-1}$)	1.628	1.652	1.678	1.708	1.740	1.774	1.811
C ($J K^{-1} mol^{-1}$)	110.9	112.5	114.3	116.3	118.5	120.9	123.4
Temp. (K)	273.15	280	290	298.15	300		
c ($J K^{-1} g^{-1}$)	1.823	1.850	1.890	1.924	1.932		
C ($J K^{-1} mol^{-1}$)	124.2	126.0	128.8	131.1	131.6		

TABLE 12.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	52	23	0.371	1.27–2	0.09	5.65–4	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
161.5–300.8	500.00	1.75463+2	1.46617+1	–3.07278	1.76862+2	–4.12338	1.77725+2	II



Name: Spiropentane
Formula: C_5H_8

CAS-RN: 157–40–4
Group No.: 12–004
Molar Mass: 68.12

TABLE 12.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
50SCO/FIN2	176.4–312.1	18	0.20	99.87	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 12.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.133	3.90–3	0.03	1.59–7	0
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
176.4–312.1	1.84093+1	–7.98160	3.35441	–3.11378–1	II

TABLE 12.4.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.598	1.613	1.632	1.655	1.681	1.710	1.742
C_{sat} (J K^{-1}mol^{-1})	108.9	109.9	111.2	112.7	114.5	116.5	118.7
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.777	1.814	1.853	1.866	1.895	1.938	1.975
C_{sat} (J K^{-1}mol^{-1})	121.0	123.6	126.2	127.1	129.1	132.0	134.5
Temp. (K)	300	310					
c_{sat} (J K^{-1}g^{-1})	1.983	2.029					
C_{sat} (J K^{-1}mol^{-1})	135.1	138.2					

TABLE 12.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.191	5.62–3	0.04	6.52–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
176.4–312.1	512.00	1.45703+2	1.17743+1	4.33588–1	1.42795+2	9.42793	1.43898+2	II

Name: Cyclopentane
Formula: C_5H_{10}

CAS–RN: 287–92–3
Group No.: 12–005
Molar Mass: 70.13

TABLE 12.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
34JAC/PAR	186.0–293.7	15	nosp	not specified	C_p	BSIO	25PAR
43AST/FIN	184.1–291.4	19	nosp	99.999 melpt	C_p	BSAO	39AST/EID1
46DOU/HUF1	185.8–300.1	16	0.20	99.995 melpt	C_p	BSAO	43RUE/HUF
47SZA/MOR	180.0–300.0	21S	0.10	not specified	C_p	BSAO	47AST/SZA
75JOL/BOI	298.1	1	0.30	99.9 melpt	C_p	FSIT	71PIC/LED
79FOR/DAR	298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
83SID/SVE	293.1	1	nosp	99.9 chrom	C_p	FSIT	71PIC/LED
85TAN	298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED

TABLE 12.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46DOU/HUF1	185.8–300.1	16	0.20#	0.606	1.55–2	0.12	9.98–3	8
47SZA/MOR	180.0–300.0	21	0.10	0.716	9.22–3	0.07	–1.89–3	–2
79FOR/DAR	298.1	1	0.30#	0.182	8.33–3	0.05	8.33–3	1
85TAN	298.1	1	0.30	0.160	7.30–3	0.05	–7.30–3	–1
				Rejected data				
34JAC/PAR	(9.27–2, 0.71, –4.29–2, –7)			43AST/FIN	(1.01–1, 0.72, 7.70–2, 11)			
75JOL/BOI	(5.76–2, 0.38, 5.76–2, 1)			83SID/SVE	(1.21–1, 0.80, 1.21–1, 1)			

TABLE 12.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	75	39	0.691	1.28–2	0.10	3.11–3	6
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.0–300.1		1.79538+1	–8.74268	3.62016	–3.32700–1		II

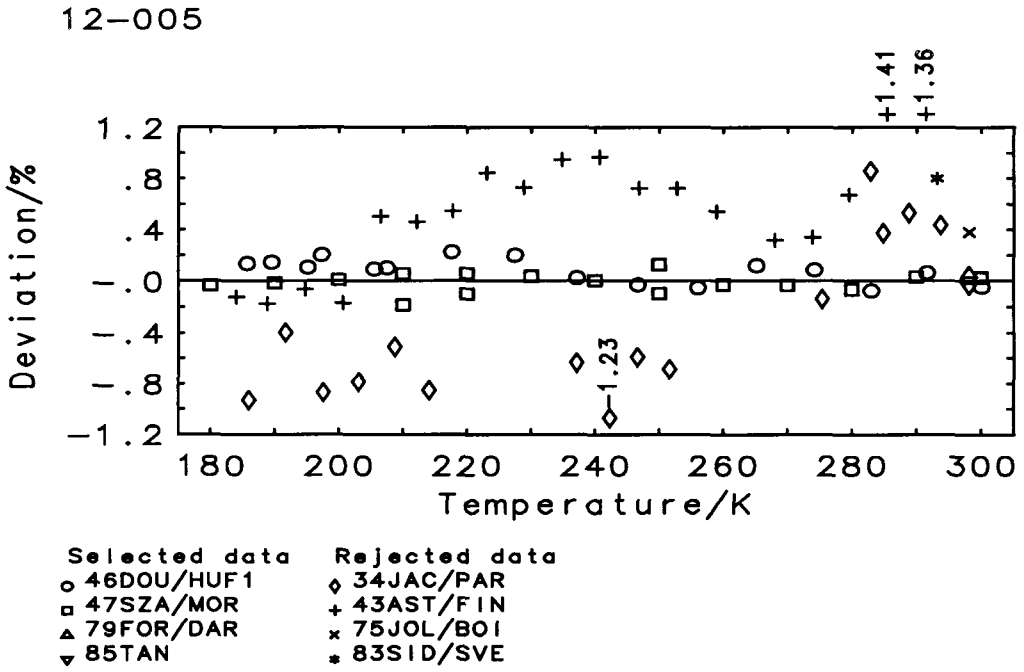
TABLE 12.5.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.423	1.438	1.457	1.479	1.505	1.535	1.568
C_p (J K^{-1}mol^{-1})	99.82	100.9	102.2	103.7	105.6	107.7	110.0
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.603	1.642	1.682	1.696	1.725	1.770	1.808
C_p (J K^{-1}mol^{-1})	112.5	115.1	118.0	118.9	121.0	124.1	126.8
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.817						
C_p (J K^{-1}mol^{-1})	127.4						

TABLE 12.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	75	39	0.837	1.27–2	0.10	–3.30–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
180.0–300.1	511.70	1.51777+2	1.21864+1	–1.13315	1.49227+2	8.25525	1.51974+2	II



Name: Cyclohexane-d_{12}
Formula: C_6D_{12}

CAS-RN: 1735-17-7
Group No.: 12-006
Molar Mass: 96.23

TABLE 12.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
66NIK/RAB	N	283.1–333.1	11S	0.30	not specified	C_p	BSAO	47SKU
80MRA/NAA	N	285.0–320.0	9	1.00	not specified	C_p	BDHT	69PER/COM

66NIK/RAB deuteration: 97 mol.%
80MRA/NAA deuterated to 99.5 mol.%, content of impurities below 0.3 mol.%

TABLE 12.6.2. Correlated heat capacities

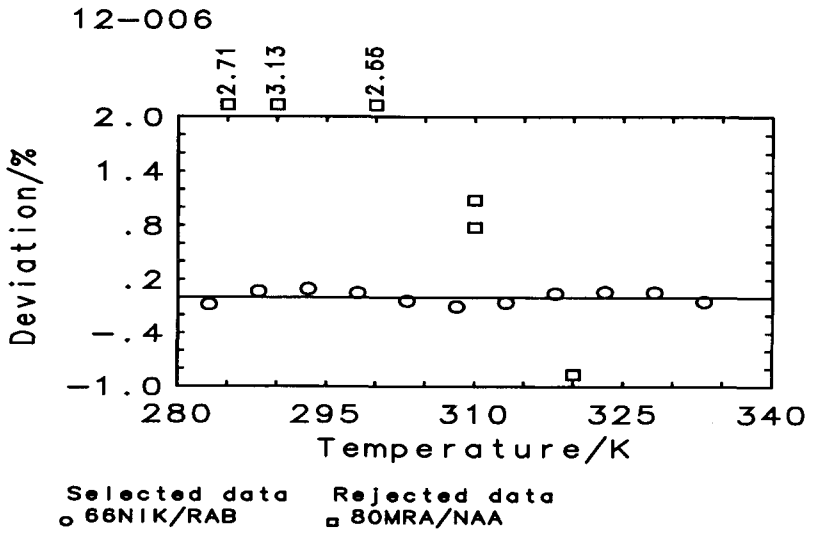
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
66NIK/RAB	283.1–333.1	11	0.30	0.223	1.52–2	0.07	1.92–5	1
				Rejected data				
80MRA/NAA	(4.95–1, 2.21, 3.58–1, 5)							

TABLE 12.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	11	0.261	1.79–2	0.08	1.92–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
283.1–333.1		5.13584+1	–2.79697+1	6.08981			IV

TABLE 12.6.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.796	1.854	1.910	1.923	2.002	2.092	2.192
C_p ($J K^{-1} mol^{-1}$)	172.8	178.4	183.8	185.1	192.7	201.3	211.0



Name: Cyclohexane
Formula: C_6H_{12}

CAS–RN: 110–82–7
Group No.: 12–007
Molar Mass: 84.16

TABLE 12.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
19DEJ		295.6–323.3	10	nosp	not specified	C_p	BSIO	19DEJ
30PAR/HUF2		283.1–298.9	5	0.30	not specified	C_p	BSIO	25PAR
39PHI		304.1	1	nosp	not specified	C_p	BSIO	49WEI
43AST/SZA		281.6–292.5	4	nosp	99.905 melpt	C_p	BSAO	39AST/EID1
43RUE/HUF		282.3–301.3	7	0.20	99.985 melpt	C_p	BSAO	43RUE/HUF
48TSC2		292.6	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC6		293.6	1	nosp	not specified	C_p	BSIO	48TSC1
50AUE/SAG		299.8–366.5	13	nosp	99.9 melpt	C_p	BSAO	39SAG/EVA
60SWI/ZIE	N	311.6–322.2	2	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
61ROU		300.4–315.8	7	nosp	99.94 anal	C_p	BSAO	61ROU
64MOE/THO		298.0–327.7	4	0.50	not specified	C_p	BSIO	64MOE/THO
66KLE		293.1–343.1	11S	0.10	not specified	C_p	BSAO	66KLE
66NIK/RAB		283.1–333.1	11S	0.30	not specified	C_p	BSAO	47SKU
68REC1	N	298.0–313.0	eqn	nosp	not specified	C_p	BSAO	68REC1
69WIL/SCH		293.1–313.1	3	0.40	not specified	C_p	BDAO	65FIN/GRU
73SUB/RAJ		298.1–323.1	3	0.30	not specified	C_p	BSIO	64MOE/THO
74WIL/ZET		283.1–323.1	5	nosp	not specified	C_p	BSAO	64ARN1
75JOL/BOI		298.1	1	0.30	99.9 melpt	C_p	FSIT	71PIC/LED
75SAN	N	398.1–523.2	9S	1.00	not specified	C_p	FSIO	75SAN
78GRO/WIL		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
78SAF		299.1–311.7	7	nosp	not specified	C_p	BSAO	67RAS/GAN
78SAF		299.1–311.7	7	nosp	not specified	C_p	FSIO	75SAF/GER
78SAF		299.1–311.7	7	nosp	not specified	C_p	BSAO	67RAS/GAN
79FOR/DAR		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
79MAR/BRA		298.1	1	1.00	not specified	C_p	BDCT	70PAZ/PAZ
79WIL/GRO		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
82GRO/ING		298.1	1	0.30	99.5 melpt	C_p	FSIT	71PIC/LED
82TAN		293.1–303.1	3S	0.30	99.99 chrom	C_p	FSIT	71PIC/LED
83SID/SVE		293.1	1	0.30	99.9 chrom	C_p	FSIT	71PIC/LED
85NKI/CHA		298.0	1	0.30	not specified	C_p	FSIT	71PIC/LED
85TAN/NAK		283.1–318.1	3	0.30	100.0 chrom	C_p	FSIT	71PIC/LED
86JIM/ROM		298.1	1	nosp	99.5 anal	C_p	FSIT	71PIC/LED
86ORT		298.1	1	1.00	99.5 anal	C_p	BDCT	70PAZ/PAZ
87KAL/KOH		293.1–313.1	2	nosp	not specified	C_p	FSIT	71PIC/LED
88SHI/OGA2		298.1	1	nosp	99.9 chrom	C_p	FSIO	85OGA
89JIM/ROU		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
90JAL/ROB		293.0	1	5.00	99. anal	C_p	BDHT	87PER/COM
91OGA/MIT		298.1	1	nosp	not specified	C_p	FSIO	85OGA
91TRE/COS		298.1	1	nosp	99.98 anal	C_p	FSIT	71PIC/LED

60SWI/ZIE average values in temperature ranges 294–329 K and 294–350 K
68REC1 same data in 68REC2
75SAN same data in 76SAN/MEL; C_p at the saturation pressure extrapolated from high pressure measurement

TABLE 12.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
43RUE/HUF	282.3–301.3	7	0.20#	0.224	8.35–3	0.04	5.52–3	4
50AUE/SAG	322.0–366.5	9	1.00#	1.154	2.41–1	1.15	–2.40–1	–9
64MOE/THO	298.0–327.7	4	0.50	0.604	5.67–2	0.30	–3.28–2	0
66KLE	293.1–343.1	11	0.10	0.502	9.91–3	0.05	–3.39–3	–3
74WIL/ZET	283.1–323.1	5	0.35#	0.930	6.25–2	0.33	6.20–2	5
75JOL/BOI	298.1	1	0.30	0.068	3.82–3	0.02	–3.82–3	–1
75SAN	398.1–523.2	9	1.00	1.266	4.50–1	1.27	1.17–2	–1
78GRO/WIL	298.1	1	0.30	0.252	1.42–2	0.08	1.42–2	1
78SAF	299.1–311.7	7	0.30	0.959	5.51–2	0.29	5.50–2	7
78SAF	299.1–311.7	7	0.70#	0.434	5.82–2	0.30	5.78–2	7
79FOR/DAR	298.1	1	0.30	0.175	9.84–3	0.05	–9.84–3	–1
79WIL/GRO	298.1	1	0.30	0.380	2.14–2	0.11	2.14–2	1
82GRO/ING	298.1	1	0.30	0.465	2.62–2	0.14	2.62–2	1
82TAN	293.1–303.1	3	0.30	0.494	2.77–2	0.15	–2.68–2	–3
85TAN/NAK	283.1–318.1	3	0.30	0.695	3.80–2	0.21	–3.27–2	–3
91OGA/MIT	298.1	1	0.30#	0.474	2.67–2	0.14	–2.67–2	–1
91TRE/COS	298.1	1	0.30#	0.495	2.79–2	0.15	–2.79–2	–1

Rejected data

19DEJ	(2.48, 11.37, 2.47, 10)	30PAR/HUF2	(2.42–1, 1.34, –2.39–1, –5)
39PHI	(7.00, 57.96, –7.00, –1)	43AST/SZA	(1.76–1, 0.95, 1.75–1, 3)
48TSC2	(7.26–2, 0.39, –7.26–2, –1)	48TSC6	(2.03–1, 1.11, –2.03–1, –1)
60SWI/ZIE	(7.29–1, 3.85, –7.29–1, –2)	61ROU	(2.05–1, 1.05, 2.05–1, 7)
66NIK/RAB	(3.33–1, 1.82, –2.05–1, –5)	68REC1	(1.53–1, 0.80, –1.46–1, –4)
69WIL/SCH	(1.42–1, 0.75, –1.39–1, –3)	73SUB/RAJ	(2.59–1, 1.34, 2.03–1, 3)
78SAF	(9.00–2, 0.47, 8.97–2, 7)	79MAR/BRA	(7.43–2, 0.40, –7.43–2, –1)
83SID/SVE	(5.85–2, 0.31, 5.85–2, 1)	85NKI/CHA	(4.39–2, 0.23, 4.39–2, 1)
86JIM/ROM	(9.96–2, 0.53, 9.96–2, 1)	86ORT	(4.59–2, 0.25, –4.59–2, –1)
87KAL/KOH	(1.99–1, 1.01, 1.81–1, 2)	88SHI/OGA2	(2.30–1, 1.24, –2.30–1, –1)
89JIM/ROU	(1.01–1, 0.53, 1.01–1, 1)	89LAI/ROD	(8.04–2, 0.43, 8.04–2, 1)
90JAL/ROB	(2.33–1, 1.27, –2.33–1, –1)		

TABLE 12.7.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	146	72	0.837	1.92–1	0.66	–1.76–2	3
C_{sat}	146	72	0.821	1.78–1	0.64	–1.76–2	2

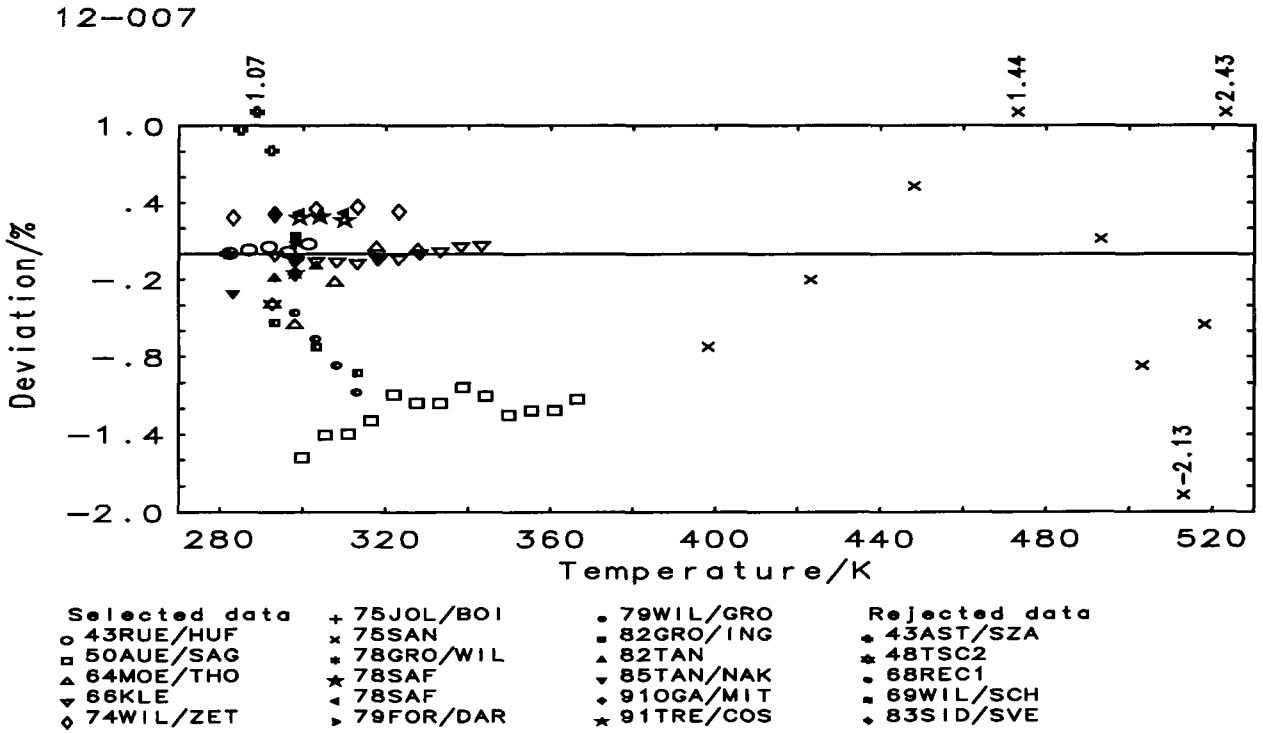
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
282.3–360.0	–2.05560+1	3.05528+1	–8.75552	9.84165–1	II
360.0–440.0	1.01668+2	–7.13008+1	1.95371+1	–1.63553	IV
440.0–523.2	–1.26591+3	8.61138+2	–1.92381+2	1.44189+1	V
282.3–360.0	–2.09531+1	3.07362+1	–8.74351	9.74511–1	II
360.0–440.0	1.03511+2	–7.29843+1	2.00677+1	–1.69320	IV
440.0–523.2	–1.06245+3	7.21990+2	–1.60608+2	1.19944+1	V

TABLE 12.7.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1}g^{-1}$)	1.774	1.819	1.856	1.865	1.910	1.957	2.004
C_p ($J K^{-1}mol^{-1}$)	149.3	153.1	156.2	156.9	160.8	164.7	168.7
c_{sat} ($J K^{-1}g^{-1}$)	1.773	1.819	1.856	1.865	1.910	1.956	2.004
C_{sat} ($J K^{-1}mol^{-1}$)	149.3	153.1	156.2	156.9	160.8	164.6	168.6
Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1}g^{-1}$)	2.054	2.106	2.162	2.220	2.282	2.345	2.409
C_p ($J K^{-1}mol^{-1}$)	172.9	177.3	181.9	186.9	192.0	197.4	202.8
c_{sat} ($J K^{-1}g^{-1}$)	2.053	2.104	2.158	2.216	2.276	2.338	2.400
C_{sat} ($J K^{-1}mol^{-1}$)	172.8	177.1	181.7	186.5	191.6	196.8	202.0
Temp. (K)	410	420	430	440	450	460	470
c_p ($J K^{-1}g^{-1}$)	2.473	2.536	2.596	2.654	2.71	2.77	2.84
C_p ($J K^{-1}mol^{-1}$)	208.1	213.4	218.5	223.4	228	233	239
c_{sat} ($J K^{-1}g^{-1}$)	2.462	2.522	2.579	2.634	2.68	2.74	2.80
C_{sat} ($J K^{-1}mol^{-1}$)	207.2	212.2	217.1	221.7	226	230	236
Temp. (K)	480	490	500	510	520		
c_p ($J K^{-1}g^{-1}$)	2.94	3.06	3.22	3.43	3.70		
C_p ($J K^{-1}mol^{-1}$)	247	258	271	289	311		
c_{sat} ($J K^{-1}g^{-1}$)	2.88	2.99	3.12	3.29	3.51		
C_{sat} ($J K^{-1}mol^{-1}$)	243	251	263	277	296		

TABLE 12.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	146	72	1.386	1.94–1	0.65	–9.47–3	–7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
282.3–523.2	553.50	–4.19042	3.31133–1	7.71652	1.32572+1		V



Name: Methylcyclopentane
Formula: C_6H_{12}

CAS-RN: 96-37-7
Group No.: 12-008
Molar Mass: 84.16

TABLE 12.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31HUF/PAR	139.0–293.7	8	1.00	not specified		C_p	BSIO	25PAR
46DOU/HUF1	136.1–307.5	31	0.20	99.907	melpt	C_p	BSAO	43RUE/HUF
51CON/SAG	299.8–366.5	13S	0.70	99.9	estim	C_p	BSAO	39SAG/EVA
83SID/SVE	293.1	1	0.30	99.9	melpt	C_p	FSIT	71PIC/LED

TABLE 12.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46DOU/HUF1	136.1–307.5	31	0.20#	0.416	1.44–2	0.08	9.70–5	–4
51CON/SAG	299.8–366.5	13	0.70	0.187	2.83–2	0.13	–2.06–3	–10
				Rejected data				
31HUF/PAR	(1.14–1, 0.71, –9.83–2, –6)			83SID/SVE	(9.69–2, 0.51, 9.69–2, 1)			

TABLE 12.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	44	0.381	2.06–2	0.10	–5.40–4	–14
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
136.1–366.5		1.86504+1	–5.70883	2.48334	–1.74291–1		III

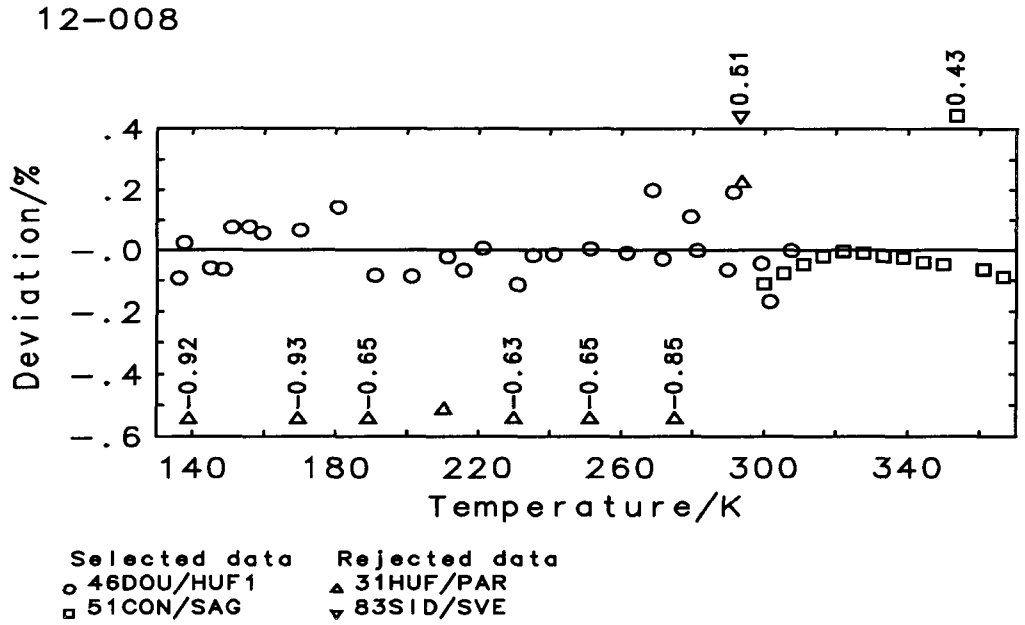
TABLE 12.8.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p (J K^{-1}g^{-1})	1.487	1.490	1.498	1.508	1.522	1.538	1.558
C_p (J K^{-1}mol^{-1})	125.1	125.4	126.0	126.9	128.1	129.5	131.1
Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.581	1.606	1.634	1.664	1.697	1.732	1.769
C_p (J K^{-1}mol^{-1})	133.0	135.1	137.5	140.0	142.8	145.8	148.9
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.782	1.809	1.850	1.885	1.894	1.939	1.986
C_p (J K^{-1}mol^{-1})	149.9	152.2	155.7	158.7	159.4	163.2	167.1
Temp. (K)	330	340	350	360	370		
c_p (J K^{-1}g^{-1})	2.034	2.084	2.136	2.188	2.242		
C_p (J K^{-1}mol^{-1})	171.2	175.4	179.7	184.2	188.7		

TABLE 12.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	44	0.681	4.50–2	0.22	2.29–3	–8

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
136.1–366.5	532.73	1.07170+2	7.53370	7.13094	1.04425+2	1.05510+1	1.19907+2	III



Name: Tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane
Formula: C_7H_8

CAS-RN: 278–06–8
Group No.: 12–009
Molar Mass: 92.14

TABLE 12.9.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73HAL/SMI	N	297.15	1.510	nosp	99.9	chrom	C_p	BDHT	71DU/COM

73HAL/SMI same data in 88CZA1 and 88CZA2

Name: Bicyclo[4.1.0]heptane
Formula: C_7H_{12}

CAS-RN: 286–08–8
Group No.: 12–010
Molar Mass: 96.17

TABLE 12.10.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70CHA/MCN	315.00	1.953	2.00	not specified		C_p	BDHT	73PER/COM

Name: Ethylidenecyclopentane
Formula: C_7H_{12}

CAS–RN: 2146–37–4
Group No.: 12–011
Molar Mass: 96.17

TABLE 12.11.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC/PEA	298.15	1.884	1.50	99.	chrom	C_p	BSIO	80FUC

Name: Methylenecyclohexane
Formula: C_7H_{12}

CAS–RN: 1192–37–6
Group No.: 12–012
Molar Mass: 96.17

TABLE 12.12.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC/PEA	298.15	1.845	1.50	99.	chrom	C_p	BSIO	80FUC

Name: Cycloheptane
Formula: C_7H_{14}

CAS–RN: 291–64–5
Group No.: 12–013
Molar Mass: 98.19

TABLE 12.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56FIN/SCO	269.3–300.4	7	0.20	99.951	melpt	C_{sat}	BSAO	43RUE/HUF
75JOL/BOI	298.1	1	0.30	99.0	melpt	C_p	FSIT	71PIC/LED
79FOR/DAR	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 12.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56FIN/SCO	269.3–300.4	7	0.20#	0.105	4.43–3	0.02	6.97–4	1
79FOR/DAR	298.1	1	0.30	0.168	1.09–2	0.05	–1.09–2	–1
				Rejected data				
75JOL/BOI	(2.78–2, 0.13, –2.78–2, –1)							

TABLE 12.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	9	8	0.133	6.54–3	0.03	–7.55–4	0
Temp. range K		A_1	A_2				Level of uncertainty
269.3–300.4		8.12315	4.56483				II

TABLE 12.13.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c ($J K^{-1}g^{-1}$)	1.732	1.744	1.770	1.809	1.840	1.848
C ($J K^{-1}mol^{-1}$)	170.0	171.2	173.8	177.6	180.7	181.4

Name: 1,1–Dimethylcyclopentane
Formula: C_7H_{14}

CAS–RN: 1638–26–2
Group No.: 12–014
Molar Mass: 98.19

TABLE 12.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53GRO/OLI	205.9–299.8	14	0.20	99.998	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 12.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	14	0.307	1.26–2	0.06	7.49–6	–2
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
205.9–299.8	2.95924+1	–1.80455+1	8.11618	–9.61125–1			II

TABLE 12.14.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} ($J K^{-1}g^{-1}$)	1.574	1.604	1.637	1.672	1.709	1.748	1.788
C_{sat} ($J K^{-1}mol^{-1}$)	154.6	157.5	160.7	164.2	167.8	171.7	175.6
Temp. (K)	273.15	280	290	298.15	300		
c_{sat} ($J K^{-1}g^{-1}$)	1.801	1.829	1.869	1.902	1.910		
C_{sat} ($J K^{-1}mol^{-1}$)	176.8	179.6	183.6	186.8	187.5		

TABLE 12.14.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	14	0.705	2.94–2	0.14	6.53–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
205.9–299.8	547.00	–6.41924	1.96454	1.02632+1	5.24382		II

Name: *cis*–1,2–Dimethylcyclopentane
Formula: C_7H_{14}

CAS–RN: 1192–18–3
Group No.: 12–015
Molar Mass: 98.19

TABLE 12.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53GRO/OLI	223.1–302.8	14	0.20	99.992	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 12.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	14	0.220	9.25–3	0.04	5.59–6	–4

Temp. range K	A_1	A_2	A_3	Level of uncertainty
223.1–302.8	1.51102+1	2.57996–1	7.68422–1	II

TABLE 12.15.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.674	1.707	1.741	1.776	1.813	1.825	1.851
C_{sat} (J K^{-1}mol^{-1})	164.4	167.6	170.9	174.4	178.0	179.2	181.7

Temp. (K)	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.890	1.923	1.931
C_{sat} (J K^{-1}mol^{-1})	185.6	188.8	189.6

TABLE 12.15.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	14	0.276	1.16–2	0.06	9.94–6	–3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
223.1–302.8	565.00	–6.42470	1.97572	1.09516+1	5.22301	II

Name: *trans*–1,2–Dimethylcyclopentane
Formula: C_7H_{14}

CAS–RN: 822–50–4
Group No.: 12–016
Molar Mass: 98.19

TABLE 12.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31HUF/PAR	N	161.5–294.2	8	1.00	not specified		C_p	BSIO	25PAR

31HUF/PAR unspecified stereoisomer or mixture; authors supposed *trans*–isomer (according to n.m.t. and n.b.t.)

TABLE 12.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.349	6.98–2	0.35	3.28–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
161.5–294.2		1.54912+1	5.64126–1	6.14681–1			V

TABLE 12.16.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.54	1.57	1.59	1.62	1.64	1.67	1.70
C_p (J K^{-1}mol^{-1})	152	154	156	159	161	164	167
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.73	1.76	1.79	1.82	1.83	1.85	1.89
C_p (J K^{-1}mol^{-1})	169	172	176	179	180	182	185
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.92	1.92					
C_p (J K^{-1}mol^{-1})	188	189					

TABLE 12.16.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.305	6.00–2	0.31	2.31–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
161.5–294.2	553.00	–5.05442	2.44579	1.20389+1	2.61135		V

Name: *trans*–1,3–Dimethylcyclopentane
Formula: C_7H_{14}

CAS–RN: 1759–58–6
Group No.: 12–017
Molar Mass: 98.19

TABLE 12.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53GRO/OLI	143.7–304.0	22	0.20	99.98	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 12.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.185	7.42–3	0.04	4.16–6	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
143.7–304.0		1.78458+1	–2.42108	1.56831	–7.17062–2		II

TABLE 12.17.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J K^{-1}g^{-1})	1.482	1.498	1.517	1.537	1.559	1.584	1.610
C_{sat} (J K^{-1}mol^{-1})	145.5	147.1	148.9	150.9	153.1	155.5	158.1
Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	1.638	1.668	1.700	1.734	1.769	1.806	1.818
C_{sat} (J K^{-1}mol^{-1})	160.9	163.8	166.9	170.2	173.7	177.4	178.5
Temp. (K)	280	290	298.15	300			
c_{sat} (J K^{-1}g^{-1})	1.845	1.885	1.920	1.927			
C_{sat} (J K^{-1}mol^{-1})	181.2	185.1	188.5	189.2			

TABLE 12.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	22	22	1.029	4.14–2	0.21	1.25–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
143.7–304.0	553.00	2.40978–1	6.69964	8.35847	2.16693–3		II

Name: Ethylcyclopentane
Formula: C_7H_{14}

CAS–RN: 1640–89–7
Group No.: 12–018
Molar Mass: 98.19

TABLE 12.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53GRO/OLI	140.2–301.8	21	0.20	99.97	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 12.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	21	21	0.171	6.66–3	0.03	1.54–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
140.2–301.8		2.12846+1	–5.96739	2.67319	–1.83805–1		II

TABLE 12.18.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.496	1.501	1.510	1.521	1.535	1.553	1.573
C_{sat} (J K^{-1}mol^{-1})	146.9	147.4	148.2	149.3	150.8	152.5	154.4
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.595	1.621	1.648	1.678	1.711	1.745	1.782
C_{sat} (J K^{-1}mol^{-1})	156.6	159.1	161.8	164.8	168.0	171.4	175.0
Temp. (K)	273.15	280	290	298.15	300		
c_{sat} (J K^{-1}g^{-1})	1.794	1.821	1.861	1.895	1.903		
C_{sat} (J K^{-1}mol^{-1})	176.1	178.8	182.7	186.1	186.9		

TABLE 12.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.192	7.66–3	0.04	2.00–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
140.2–301.8	569.50	4.42530+2	4.37635+1	–2.67447+1	4.09232+2	1.01638+2	3.01333+2	II

Name: Methylcyclohexane
Formula: C_7H_{14}

CAS–RN: 108–87–2
Group No.: 12–019
Molar Mass: 98.19

TABLE 12.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF1	151.4–294.2	12	1.00	not specified		C_p	BSIO	25PAR
46DOU/HUF1	155.1–285.8	15	0.20	99.989	melpt	C_p	BSAO	43RUE/HUF
48TSC2	292.6	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC6	293.6	1	nosp	not specified		C_p	BSIO	48TSC1
66HWA/ZIE	174.8–308.1	32	nosp	99.0	melpt	C_p	BSAO	45SCO/MEY
75HOL/ZIE	144.0–312.0	eqn	0.20	99.88	anal	C_p	BSAO	45SCO/MEY
79WIL/GRO	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
82GRO/ING	298.1	1	0.30	99.5	estim	C_p	FSIT	71PIC/LED
83SID/SVE	293.1	1	0.30	99.9	chrom	C_p	FSIT	71PIC/LED
85TAN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
88SHI/OGA2	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 12.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46DOU/HUF1	155.1–285.8	15	0.20#	0.583	2.09–2	0.12	5.56–3	2
66HWA/ZIE	174.8–308.1	32	0.20#	0.583	2.23–2	0.12	1.26–2	19
75HOL/ZIE	144.0–309.0	34	0.20	0.410	1.49–2	0.08	–1.42–2	–34
85TAN	298.1	1	0.30	0.021	1.37–3	0.01	1.37–3	0
				Rejected data				
30PAR/HUF1	(7.51–2, 0.38, –3.55–2, –2)			48TSC2	(7.81–2, 0.36, –7.81–2, –1)			
48TSC6	(7.87–2, 0.36, –7.87–2, –1)			79WIL/GRO	(2.39–2, 0.11, –2.39–2, –1)			
82GRO/ING	(4.11–2, 0.18, 4.11–2, 1)			83SID/SVE	(1.24–1, 0.56, 1.24–1, 1)			
88SHI/OGA2	(6.84–2, 0.31, –6.84–2, –1)							

TABLE 12.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	100	82	0.524	1.95–2	0.10	5.87–5	–1 3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
144.0–309.0		1.57165+1	–7.17916–1	9.75107–1			II

TABLE 12.19.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.425	1.445	1.466	1.489	1.513	1.540	1.567
C_p (J K^{-1}mol^{-1})	140.0	141.9	144.0	146.2	148.6	151.2	153.9
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.597	1.628	1.661	1.695	1.731	1.769	1.781
C_p (J K^{-1}mol^{-1})	156.8	159.8	163.0	166.4	170.0	173.7	174.9
Temp. (K)	280	290	298.15	300	310		
c_p (J K^{-1}g^{-1})	1.808	1.849	1.884	1.892	1.936		
C_p (J K^{-1}mol^{-1})	177.5	181.5	184.9	185.7	190.1		

TABLE 12.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	100	82	0.674	2.61–2	0.14	–2.39–3	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
144.0–309.0	572.20	–2.64050	5.81048	8.03223	2.99985–1		II

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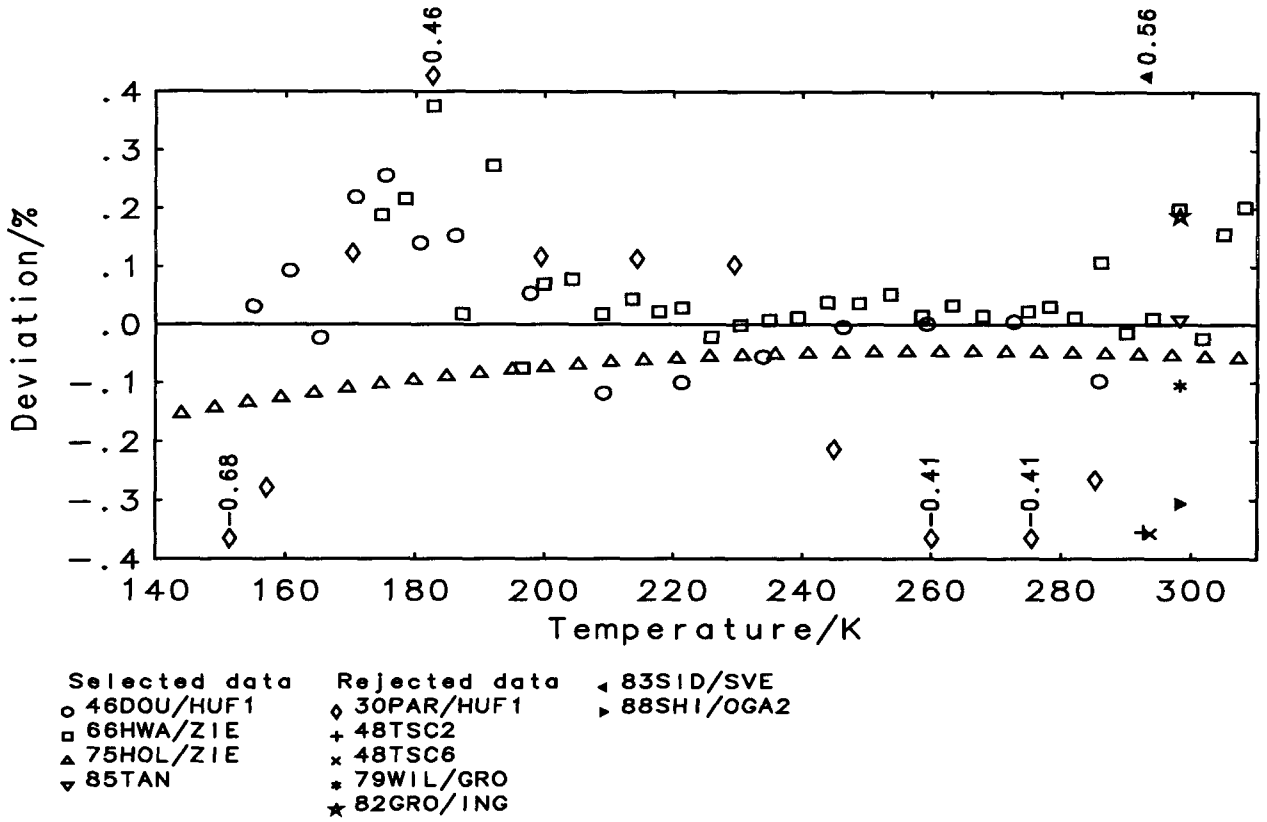


Name: Bicyclo[2.2.2]octane
Formula: C_8H_{14}

CAS-RN: 280-33-1
Group No.: 12-020
Molar Mass: 110.20

TABLE 12.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70WON/WES	450.6–482.1	10	nosp	not specified		C_{sat}	BSAO	68WES/FUR

TABLE 12.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	10	10	0.856	8.29-2	0.26	3.49-4	2
Temp. range K		A_1	A_2				Level of uncertainty
450.6–482.1		5.46925	5.76028				III

TABLE 12.20.4. Recommended values of heat capacities

Temp. (K)	450	460	470	480
c_{sat} (J K^{-1}g^{-1})	2.368	2.412	2.455	2.499
C_{sat} (J K^{-1}mol^{-1})	261.0	265.8	270.6	275.4

Name: *cis*–Bicyclo[4.2.0]octane
Formula: C_8H_{14}

CAS–RN: 28282–35–1
Group No.: 12–021
Molar Mass: 110.20

TABLE 12.21.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70CHA/MCN	345.00	2.346	2.00	not specified		C_p	BDHT	73PER/COM

Name: Ethylidenecyclohexane
Formula: C_8H_{14}

CAS–RN: 1003–64–1
Group No.: 12–022
Molar Mass: 110.20

TABLE 12.22.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC/PEA	298.15	1.849	1.50	99.	chrom	C_p	BSIO	80FUC

Name: *endo*–2–Methylbicyclo[2.2.1]heptane
Formula: C_8H_{14}

CAS–RN: 765–90–2
Group No.: 12–023
Molar Mass: 110.20

TABLE 12.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64SER/GOR	280.0–310.0	5S	nosp	99.74	melpt	C_p	BSAO	62KOL/SER

TABLE 12.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.008	9.01–4	0.00	–3.82–7	0
Temp. range K		A_1	A_2				Level of uncertainty
280.0–310.0		5.65347	5.53641				IV

TABLE 12.23.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	1.596	1.638	1.672	1.680	1.721
C_p ($J K^{-1}mol^{-1}$)	175.9	180.5	184.3	185.1	189.7

Name: *exo*–2–Methylbicyclo[2.2.1]heptane
Formula: C_8H_{14}

CAS–RN: 872–78–6
Group No.: 12–024
Molar Mass: 110.20

TABLE 12.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
64SER/GOR	N	170.0–310.0	16S	nosp	not specified	C_p	BSAO	62KOL/SER

64SER/GOR authors expect impurities of 0.2–0.3 mol.%

TABLE 12.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.100	9.26–3	0.05	8.11–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
170.0–310.0		2.03398+1	–7.56553	3.69354	–3.11857–1		IV

TABLE 12.24.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J\,K^{-1}g^{-1}$)	1.254	1.273	1.295	1.319	1.347	1.377	1.410
C_p ($J\,K^{-1}mol^{-1}$)	138.2	140.3	142.7	145.4	148.4	151.8	155.3
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J\,K^{-1}g^{-1}$)	1.445	1.482	1.521	1.562	1.575	1.605	1.649
C_p ($J\,K^{-1}mol^{-1}$)	159.2	163.3	167.6	172.1	173.6	176.8	181.7
Temp. (K)	298.15	300	310				
c_p ($J\,K^{-1}g^{-1}$)	1.686	1.695	1.742				
C_p ($J\,K^{-1}mol^{-1}$)	185.8	186.8	192.0				

Name: *cis*–Octahydropentalene
Formula: C_8H_{14}

CAS–RN: 1755–05–1
Group No.: 12–025
Molar Mass: 110.20

TABLE 12.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
70CHA/MCN	308.0–334.0	2	2.00	not specified	C_p	BDHT	73PER/COM

TABLE 12.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
308.0–334.0		5.39602	6.58053				V

TABLE 12.25.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.946	1.996	2.046
C_p ($J\,K^{-1}mol^{-1}$)	214.5	219.9	225.4

Name: *trans*–Octahydropentalene
Formula: C_8H_{14}

CAS–RN: 5597–89–7
Group No.: 12–026
Molar Mass: 110.20

TABLE 12.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70CHA/MCN	308.0–334.0	2	2.00	not specified		C_p	BDHT	73PER/COM

TABLE 12.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
308.0–334.0		−1.34823+1	1.14192+1				V

TABLE 12.26.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.65	1.74	1.83
C_p ($J\,K^{-1}mol^{-1}$)	182	192	201

Name: (2–Propenyl)cyclopentane
Formula: C_8H_{14}

CAS–RN: 3524–75–2
Group No.: 12–027
Molar Mass: 110.20

TABLE 12.27.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79FUC/PEA	298.15	1.841	1.50	99.	chrom	C_p	BSIO	80FUC

Name: Cyclooctane
Formula: C_8H_{16}

CAS–RN: 292–64–8
Group No.: 12–028
Molar Mass: 112.22

TABLE 12.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56FIN/SCO	294.6–321.6	6	0.20	99.82	melpt	C_{sat}	BSAO	43RUE/HUF
75JOL/BOI	298.1	1	0.30	99.7	melpt	C_p	FSIT	71PIC/LED
79FOR/DAR	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
79WIL/FAR	298.1	1	0.30	99.0	melpt	C_p	FSIT	71PIC/LED
85TAN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
88SHI/OGA2	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 12.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56FIN/SCO	294.6–321.6	6	0.20#	0.186	9.76–3	0.04	–5.19–4	2
79FOR/DAR	298.1	1	0.30	0.008	6.41–4	0.00	–6.41–4	0
85TAN	298.1	1	0.30	0.100	7.78–3	0.03	7.78–3	1
				Rejected data				
75JOL/BOI	(1.47–1, 0.57, –1.47–1, –1)			79WIL/FAR	(1.12–1, 0.44, –1.12–1, –1)			
88SHI/OGA2	(3.78–2, 0.15, 3.78–2, 1)							

TABLE 12.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	11	8	0.191	1.03–2	0.04	5.02–4	3
Temp. range K		A_1	A_2				Level of uncertainty
294.6–321.6		1.02950+1	5.23878				II

TABLE 12.28.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c ($J K^{-1} g^{-1}$)	1.888	1.920	1.927	1.966	2.005
C ($J K^{-1} mol^{-1}$)	211.9	215.5	216.3	220.6	225.0

Name: 1,1–Dimethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 590–66–9
Group No.: 12–029
Molar Mass: 112.22

TABLE 12.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49HUF/TOD	242.7–303.5	13	0.20	99.97	melpt	C_p	BSAO	47HUF

TABLE 12.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.202	9.46–3	0.04	4.84–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
242.7–303.5		1.61860+1	9.75223–2	9.77710–1			II

TABLE 12.29.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.670	1.708	1.747	1.760	1.787	1.829	1.865
C_p (J K^{-1}mol^{-1})	187.4	191.6	196.0	197.4	200.6	205.3	209.3
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.873						
C_p (J K^{-1}mol^{-1})	210.2						

TABLE 12.29.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.205	9.56–3	0.04	5.43–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
242.7–303.5	585.80	–8.35188	2.83840	1.03202+1	6.14379		II

Name: *cis*–1,2–Dimethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 2207–01–4
Group No.: 12–030
Molar Mass: 112.22

TABLE 12.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49HUF/TOD	228.3–298.8	16	0.20	99.9979	melpt	C_p	BSAO	47HUF

TABLE 12.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.328	1.49–2	0.07	1.60–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
228.3–298.8		1.80627+1	–7.56275–1	1.06595			II

TABLE 12.30.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.627	1.659	1.692	1.727	1.763	1.775	1.801
C_p (J K^{-1}mol^{-1})	182.6	186.1	189.9	193.7	197.8	199.1	202.1
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	1.840	1.873	1.881				
C_p (J K^{-1}mol^{-1})	206.5	210.2	211.1				

TABLE 12.30.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.325	1.47–2	0.06	1.43–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
228.3–298.8	601.00	–6.35113	4.95764	1.00864+1	2.03408		II

Name: *trans*–1,2–Dimethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 6876–23–9
Group No.: 12–031
Molar Mass: 112.22

TABLE 12.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49HUF/TOD	183.7–301.4	27	0.20	99.995	melpt	C_p	BSAO	47HUF

TABLE 12.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	27	0.170	7.60–3	0.03	3.67–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
183.7–301.4		1.86498+1	–1.70433	1.30736			II

TABLE 12.31.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1}g^{-1}$)	1.492	1.517	1.544	1.573	1.604	1.637	1.672
C_p ($J K^{-1}mol^{-1}$)	167.4	170.2	173.2	176.5	180.0	183.7	187.6
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.708	1.747	1.760	1.788	1.830	1.866	1.875
C_p ($J K^{-1}mol^{-1}$)	191.7	196.0	197.5	200.6	205.4	209.4	210.4

TABLE 12.31.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	27	0.380	1.73–2	0.08	1.86–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
183.7–301.4	591.60	–8.60285–1	8.86336	6.72416	2.08750–2		II

Name: *cis*–1,3–Dimethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 638–04–0
Group No.: 12–032
Molar Mass: 112.22

TABLE 12.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49HUF/TOD	204.2–299.5	18	0.20	99.995	melpt	C_p	BSAO	47HUF

TABLE 12.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.489	2.21–2	0.10	2.93–5	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
204.2–299.5		1.75729+1	–7.94236–1	1.12319			II

TABLE 12.32.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1}g^{-1}$)	1.545	1.575	1.607	1.640	1.675	1.712	1.750
C_p ($J K^{-1}mol^{-1}$)	173.4	176.8	180.3	184.1	188.0	192.1	196.4
Temp. (K)	273.15	280	290	298.15	300		
c_p ($J K^{-1}g^{-1}$)	1.762	1.790	1.831	1.866	1.875		
C_p ($J K^{-1}mol^{-1}$)	197.7	200.8	205.5	209.4	210.3		

TABLE 12.32.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	18	18	0.599	2.69–2	0.12	5.02–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
204.2–299.5	586.60	-6.04943	5.16520	9.49600	1.77126		II

Name: *trans*-1,3-Dimethylcyclohexane
Formula: C_8H_{16}

CAS-RN: 2207-03-6
Group No.: 12-033
Molar Mass: 112.22

TABLE 12.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49HUF/TOD	187.6–299.0	30	0.20	99.99	melpt	C_p	BSAO	47HUF

TABLE 12.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	30	30	0.254	1.13–2	0.05	1.13–5	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
187.6–299.0		1.90500+1	-1.38442	1.20050			II

TABLE 12.33.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1} g^{-1}$)	1.538	1.562	1.588	1.616	1.646	1.678	1.711
C_p ($J K^{-1} mol^{-1}$)	172.6	175.3	178.2	181.4	184.7	188.3	192.0
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.746	1.783	1.795	1.822	1.862	1.896	1.904
C_p ($J K^{-1} mol^{-1}$)	195.9	200.1	201.4	204.4	209.0	212.8	213.7

TABLE 12.33.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	30	30	0.304	1.37–2	0.06	1.35–5	-1 1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
187.6–299.0	593.20	-1.54221	8.10594	8.20165	7.33545–2		II

Name: *cis*–1,4–Dimethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 624–29–3
Group No.: 12–034
Molar Mass: 112.22

TABLE 12.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49HUF/TOD	189.5–303.2	22	0.20	99.995	melpt	C_p	BSAO	47HUF

TABLE 12.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.266	1.25–2	0.05	6.85–6	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
189.5–303.2	2.11664+1	–2.84248	1.44287	II

TABLE 12.34.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.554	1.575	1.597	1.622	1.649	1.679	1.710
C_p (J K^{-1}mol^{-1})	174.4	176.7	179.3	182.1	185.1	188.4	191.9
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.743	1.779	1.791	1.817	1.857	1.891	1.899
C_p (J K^{-1}mol^{-1})	195.6	199.6	200.9	203.9	208.3	212.2	213.1

TABLE 12.34.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.530	2.48–2	0.11	4.02–5	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
189.5–303.2	593.00	6.14959	1.17733+1	5.74797	8.03033–1	II

Name: *trans*–1,4–Dimethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 2207–04–7
Group No.: 12–035
Molar Mass: 112.22

TABLE 12.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49HUF/TOD	242.2–299.3	9	0.20	99.995	melpt	C_p	BSAO	47HUF

TABLE 12.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.309	1.42–2	0.06	1.23–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
242.2–299.3		2.13562+1	–3.12542	1.49133			II

TABLE 12.35.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.663	1.694	1.727	1.763	1.774	1.800	1.840
C_p (J K^{-1}mol^{-1})	186.6	190.1	193.8	197.8	199.1	202.0	206.5
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.874	1.882					
C_p (J K^{-1}mol^{-1})	210.3	211.2					

TABLE 12.35.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.320	1.47–2	0.06	1.36–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
242.2–299.3	587.70	–1.43304	7.61948	8.78229	6.73799–2		II

Name: Ethylcyclohexane
Formula: C_8H_{16}

CAS–RN: 1678–91–7
Group No.: 12–036
Molar Mass: 112.22

TABLE 12.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49HUF/TOD	167.4–299.2	21	0.20	99.996	melpt	C_p	BSAO	47HUF
49PAR/MOO	160.0–300.0	15S	1.00	99.1	melpt	C_p	BSIO	25PAR

TABLE 12.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
49HUF/TOD	167.4–299.2	21	0.20#	0.194	8.32–3	0.04	1.54–6	–3
				Rejected data				
49PAR/MOO	(1.06–1, 0.45, 3.59–2, 4)							

TABLE 12.36.3. Parameters of regression polynomial

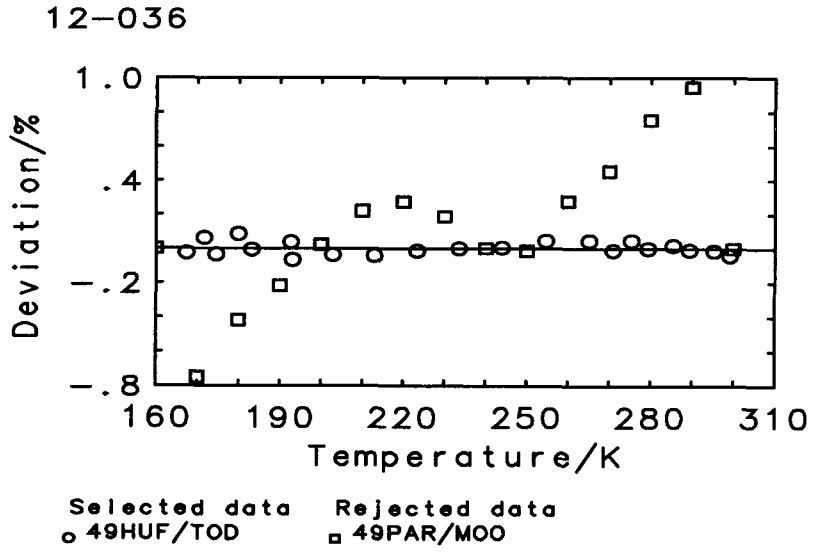
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	36	21	0.210	8.99–3	0.04	1.54–6	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
167.4–299.2		1.82969+1	–1.18127	1.20478			II

TABLE 12.36.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1} g^{-1}$)	1.465	1.487	1.512	1.538	1.566	1.595	1.627
C_p ($J K^{-1} mol^{-1}$)	164.4	166.9	169.6	172.6	175.7	179.0	182.5
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	1.660	1.695	1.732	1.770	1.783	1.810	1.853
C_p ($J K^{-1} mol^{-1}$)	186.3	190.2	194.3	198.6	200.0	203.2	207.9
Temp. (K)	298.15	300					
c_p ($J K^{-1} g^{-1}$)	1.888	1.897					
C_p ($J K^{-1} mol^{-1}$)	211.9	212.8					

TABLE 12.36.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	36	21	0.524	2.35–2	0.10	3.41–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
167.4–299.2	602.40	–2.84865–1	9.64722	6.21621	2.10289–3		II



Name: Propylcyclopentane
Formula: C_8H_{16}

CAS–RN: 2040–96–2
Group No.: 12–037
Molar Mass: 112.22

TABLE 12.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65MES/TOD1	162.1–364.6	25	0.20	99.95	melpt	C_{sat}	BSAO	47HUF

TABLE 12.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.593	2.73–2	0.12	5.52–5	–4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
162.1–364.6	2.61195+1	–8.71538	3.97711	–3.57738–1	II

TABLE 12.37.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.548	1.559	1.573	1.590	1.610	1.633	1.659
C_{sat} (J K^{-1}mol^{-1})	173.7	174.9	176.5	178.5	180.7	183.3	186.1
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.686	1.716	1.749	1.783	1.818	1.830	1.856
C_{sat} (J K^{-1}mol^{-1})	189.2	192.6	196.2	200.0	204.0	205.3	208.2
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.894	1.927	1.934	1.976	2.018	2.061	2.104
C_{sat} (J K^{-1}mol^{-1})	212.6	216.2	217.1	221.7	226.4	231.3	236.1
Temp. (K)	350	360	370				
c_{sat} (J K^{-1}g^{-1})	2.149	2.193	2.238				
C_{sat} (J K^{-1}mol^{-1})	241.1	246.1	251.1				

TABLE 12.37.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.699	3.24–2	0.14	5.61–5	–6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
162.1–364.6	596.20	2.55862+2	2.21400+1	–2.00627	2.36140+2	7.57297+1	1.92612+2	II

Name: *cis*–Bicyclo[6.1.0]nonane
Formula: C_9H_{16}

CAS–RN: 13757–43–2
Group No.: 12–038
Molar Mass: 124.23

TABLE 12.38.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70CHA/MCN	315.00	1.893	2.00	not specified		C_p	BDHT	73PER/COM

Name: Octahydro–1*H*–indene
Formula: C_9H_{16}

CAS–RN: 496–10–6
Group No.: 12–039
Molar Mass: 124.23

TABLE 12.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–423.1	3	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.095	2.72–2	0.10	5.18–3	1
63GUD/CAM	313.1–423.1	3	1.00#	0.101	2.88–2	0.10	–5.03–3	–1

TABLE 12.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.139	3.96–2	0.14	7.18–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–423.1		6.64917+1	–2.83722+1	4.98570			IV

TABLE 12.39.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	1.770	1.791	1.818	1.851	1.892	1.939	1.992
C_p ($J K^{-1}mol^{-1}$)	219.9	222.4	225.8	230.0	235.0	240.8	247.5
Temp. (K)	380	390	400	410	420		
c_p ($J K^{-1}g^{-1}$)	2.053	2.120	2.194	2.274	2.361		
C_p ($J K^{-1}mol^{-1}$)	255.0	263.3	272.5	282.5	293.3		

Name: *cis*–Octahydro–1*H*–indene
Formula: C_9H_{16}

CAS–RN: 4551–51–3
Group No.: 12–040
Molar Mass: 124.23

TABLE 12.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72FIN/MCC	239.4–366.7	17	0.20	99.989	melpt	C_{sat}	BSAO	47HUF

TABLE 12.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.143	7.49–3	0.03	1.23–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
239.4–366.7		2.53888+1	–9.93412	4.61579	–4.16499–1		II

TABLE 12.40.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.498	1.532	1.569	1.608	1.620	1.648	1.689
C_{sat} (J K^{-1}mol^{-1})	186.0	190.4	194.9	199.7	201.2	204.7	209.9
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.724	1.732	1.777	1.822	1.868	1.914	1.961
C_{sat} (J K^{-1}mol^{-1})	214.2	215.2	220.7	226.3	232.0	237.8	243.7
Temp. (K)	360						
c_{sat} (J K^{-1}g^{-1})	2.009						
C_{sat} (J K^{-1}mol^{-1})	249.6						

TABLE 12.40.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.576	3.02–2	0.12	5.73–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
239.4–366.7	659.00	–1.13270+1	2.68298	8.63717	1.19551+1		II

Name: *trans*–Octahydro–1*H*–indene
Formula: C_9H_{16}

CAS–RN: 3296–50–2
Group No.: 12–041
Molar Mass: 124.23

TABLE 12.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72FIN/MCC	211.9–391.0	25	0.20	99.978	melpt	C_{sat}	BSAO	47HUF

TABLE 12.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.167	8.15–3	0.03	3.13–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
211.9–391.0		2.65175+1	–1.00744+1	4.29136	–3.55052–1		II

TABLE 12.41.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	1.429	1.454	1.482	1.513	1.546	1.580	1.592
C_{sat} (J K^{-1}mol^{-1})	177.5	180.7	184.2	187.9	192.0	196.3	197.7
Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.617	1.655	1.688	1.695	1.737	1.780	1.824
C_{sat} (J K^{-1}mol^{-1})	200.9	205.6	209.7	210.6	215.8	221.1	226.5
Temp. (K)	340	350	360	370	380	390	
c_{sat} (J K^{-1}g^{-1})	1.869	1.914	1.961	2.008	2.056	2.104	
C_{sat} (J K^{-1}mol^{-1})	232.1	237.8	243.6	249.5	255.4	261.4	

TABLE 12.41.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.283	1.46–2	0.06	1.73–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
211.9–391.0	649.00	2.21586+2	1.77407+1	8.68620–1	2.04168+2	8.25614+1	1.71172+2	II

Name: (2–Propenyl)cyclohexane
Formula: C_9H_{16}

CAS–RN: 2114–42–3
Group No.: 12–042
Molar Mass: 124.23

TABLE 12.42.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79FUC/PEA	298.15	1.879	1.50	99.	chrom	C_p	BSIO	80FUC

Name: Butylcyclopentane
Formula: C_9H_{18}

CAS-RN: 2040-95-1
Group No.: 12-043
Molar Mass: 126.24

TABLE 12.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65MES/TOD1	167.9–367.6	24	0.20	99.98	melpt	C_{sat}	BSAO	47HUF

TABLE 12.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.170	9.33–3	0.03	5.25–6	1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
167.9–367.6	3.23222+1	−1.21006+1	5.18240	−4.83250−1			II

TABLE 12.43.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.604	1.615	1.628	1.646	1.666	1.689	1.714
C_{sat} (J K^{-1}mol^{-1})	202.5	203.8	205.6	207.7	210.3	213.2	216.4
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.742	1.772	1.805	1.839	1.850	1.875	1.912
C_{sat} (J K^{-1}mol^{-1})	219.9	223.7	227.8	232.1	233.5	236.7	241.4
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.943	1.950	1.990	2.031	2.072	2.114	2.156
C_{sat} (J K^{-1}mol^{-1})	245.3	246.2	251.2	256.4	261.6	266.9	272.2
Temp. (K)	360	370					
c_{sat} (J K^{-1}g^{-1})	2.198	2.241					
C_{sat} (J K^{-1}mol^{-1})	277.5	282.9					

TABLE 12.43.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.323	1.81–2	0.06	4.85–6	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
167.9–367.6	621.20	5.23910+2	5.08852+1	−2.74838+1	4.81266+2	1.38362+2	3.51213+2	II

Name: Propylcyclohexane
Formula: C_9H_{18}

CAS-RN: 1678–92–8
Group No.: 12–044
Molar Mass: 126.24

TABLE 12.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65FIN/MES	185.5–373.2	24	0.20	99.96	melpt	C_{sat}	BSAO	47HUF

TABLE 12.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.094	5.68–3	0.02	2.46–6	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
185.5–373.2	2.60337+1	–7.47579	3.93610	–3.62869–1	II

TABLE 12.44.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.551	1.576	1.603	1.632	1.663	1.696	1.731
C_{sat} (J K^{-1}mol^{-1})	195.8	198.9	202.3	206.0	209.9	214.1	218.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.767	1.805	1.817	1.844	1.884	1.918	1.925
C_{sat} (J K^{-1}mol^{-1})	223.1	227.8	229.4	232.8	237.8	242.1	243.1
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	1.968	2.011	2.054	2.098	2.142	2.187	2.231
C_{sat} (J K^{-1}mol^{-1})	248.4	253.8	259.3	264.9	270.5	276.1	281.7

TABLE 12.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.153	8.58–3	0.03	–8.74–7	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
185.5–373.2	625.60	2.08062+2	1.75359+1	3.18405	1.90809+2	9.49718+1	1.34979+2	II

Name: 6,6–Dimethyl–2–methylenebicyclo[3.1.1]heptane
Formula: $C_{10}H_{16}$

CAS-RN: 127–91–3
Group No.: 12–045
Molar Mass: 136.24

TABLE 12.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81BER/OGI	243.1–303.1	3S	nosp	not specified		C_{avg}	DSIO	*79BER

TABLE 12.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.002	2.80–3	0.01	1.27–6	0
Temp. range K		A_1	A_2				Level of uncertainty
243.1–303.1		2.51898+1	4.05602				VI

TABLE 12.45.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1}g^{-1}$)	2.13	2.16	2.18	2.21	2.21	2.23	2.26
C ($J K^{-1}mol^{-1}$)	290	294	297	300	302	304	307
Temp. (K)	298.15	300					
c ($J K^{-1}g^{-1}$)	2.28	2.28					
C ($J K^{-1}mol^{-1}$)	310	311					

Name: 4–Methylene–1–(1–methylethyl)bicyclo[3.1.0]hexane
Formula: $C_{10}H_{16}$

CAS-RN: 3387–41–5
Group No.: 12–046
Molar Mass: 136.24

TABLE 12.46.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33KOL/UDO	N	296.99	1.852	nosp	not specified		C_p	BSIT	34KOL/UDO2

33KOL/UDO same datum in 34KOL/UDO2

Name: Octahydro–4,7–methano–1*H*–indene
Formula: $C_{10}H_{16}$

CAS-RN: 6004–38–2
Group No.: 12–047
Molar Mass: 136.24

TABLE 12.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71BOY/SAN	372.0–390.0	2	nosp	99.9	melpt	C_p	BDHT	73PER/COM

TABLE 12.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
372.0–390.0		5.58572	7.54824				V

TABLE 12.47.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_p (J K^{-1}g^{-1})	2.05	2.09	2.14
C_p (J K^{-1}mol^{-1})	279	285	291

Name: 1,1'–Bicyclopentyl
Formula: $C_{10}H_{18}$

CAS-RN: 1636–39–1
Group No.: 12–048
Molar Mass: 138.25

TABLE 12.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL		310.9–422.0	3	nosp	98.9	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	not specified		C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	not specified		C_p	BDHT	63GUD/CAM
76GOO/LEE		298.1	1	nosp	99.96	melpt	C_p	not specified	

63GUD/CAM substance contained 0.01 % Cyclopentyl bromide
63GUD/CAM substance contained 0.10 % Cyclopentyl bromide

TABLE 12.48.2. Correlated heat capacities

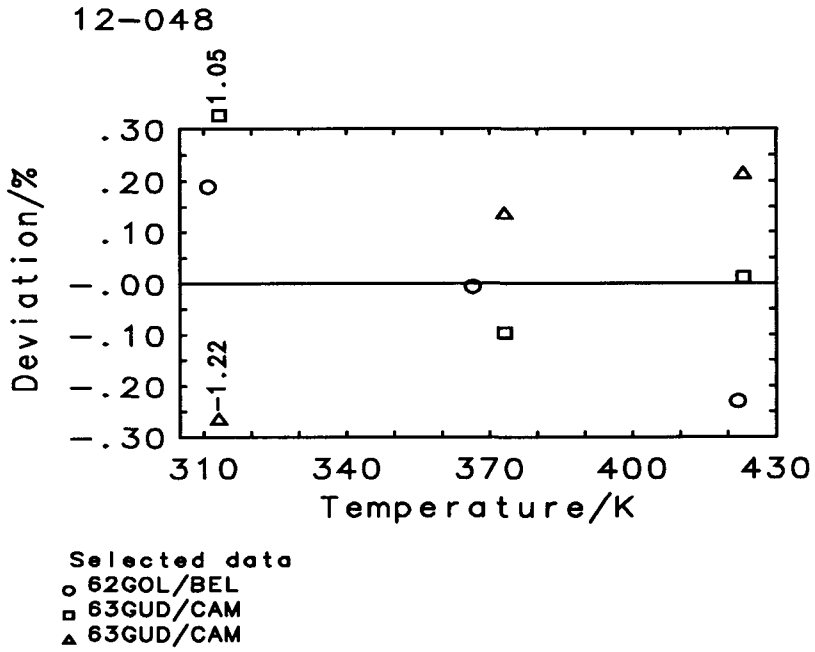
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.172	5.51–2	0.17	–1.03–2	0
63GUD/CAM	313.1–423.1	3	1.00#	0.609	1.70–1	0.61	8.87–2	0
63GUD/CAM	313.1–423.1	3	1.00#	0.720	1.98–1	0.72	–7.33–2	1

TABLE 12.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	9	0.678	1.89–1	0.68	1.70–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–423.1		6.44337+1	–2.52925+1	4.32120			IV

TABLE 12.48.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.657	1.669	1.686	1.708	1.735	1.767	1.805
C_p (J K^{-1}mol^{-1})	229.1	230.7	233.0	236.1	239.8	244.3	249.5
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	1.848	1.896	1.949	2.007	2.071		
C_p (J K^{-1}mol^{-1})	255.4	262.1	269.4	277.5	286.3		



Name: *cis*–Decahydroazulene
Formula: $C_{10}H_{18}$

CAS-RN: 16189–46–1
Group No.: 12–049
Molar Mass: 138.25

TABLE 12.49.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
70CHA/MCN	377.00	2.252	2.00	not specified	C_p	BDHT	73PER/COM

Name: Decahydronaphthalene
Formula: $C_{10}H_{18}$

CAS-RN: 91–17–8
Group No.: 12–050
Molar Mass: 138.25

TABLE 12.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
22HER/SCH		289.6	1	nosp	not specified	C_p	DSIO	22HER/SCH
62GOL/BEL	N	310.9–422.0	3	nosp	94.9 chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	not specified	C_p	BDHT	63GUD/CAM

62GOL/BEL mixture of isomers
63GUD/CAM mixture of isomers

TABLE 12.50.2. Correlated heat capacities

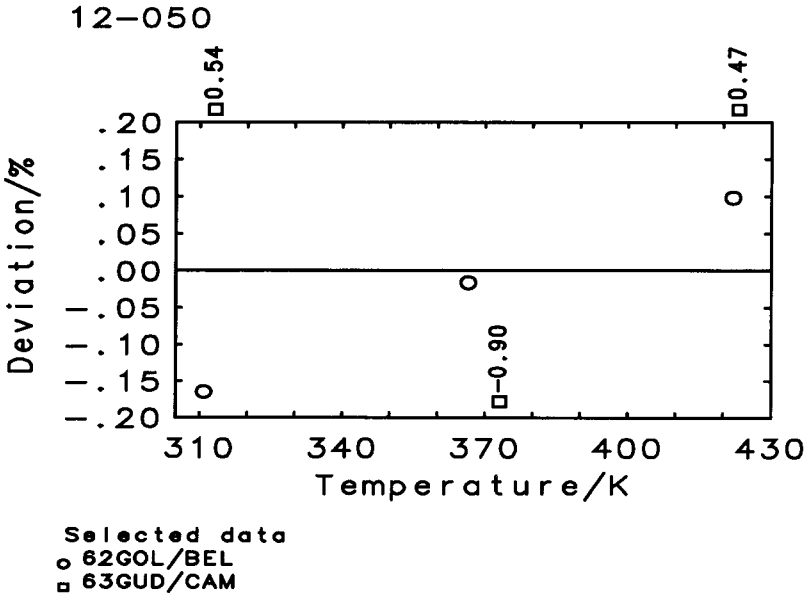
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.112	3.20–2	0.11	–5.51–3	–1
63GUD/CAM	313.1–423.1	3	1.00#	0.664	2.03–1	0.66	9.79–3	1

TABLE 12.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.583	1.78–1	0.58	2.14–3	0
Temp. range K		A_1	A_2				Level of uncertainty
310.9–423.1		4.04425	7.19381				IV

TABLE 12.50.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.584	1.628	1.671	1.714	1.757	1.801	1.844
C_p (J K^{-1}mol^{-1})	219.0	225.0	231.0	237.0	243.0	249.0	254.9
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	1.887	1.930	1.974	2.017	2.060		
C_p (J K^{-1}mol^{-1})	260.9	266.9	272.9	278.9	284.8		



Name: *cis*–Decahydronaphthalene
Formula: $C_{10}H_{18}$

CAS-RN: 493–01–6
Group No.: 12–051
Molar Mass: 138.25

TABLE 12.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49PAR/HAT		230.0–298.2	8S	0.70	99.6	melpt	C_p	BSIO	25PAR
53SEY	N	293.1–343.1	6S	nosp	not specified		C_p	BSAO	24WIL/DAN
57MCC/FIN2		234.2–344.5	37	0.20	99.88	melpt	C_{sat}	BSAO	47HUF
63GUD/CAM		313.1–423.1	3S	nosp	99.4	melpt	C_p	BDHT	63GUD/CAM
88SHI/OGA1		298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA
89OHN/FUJ		298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

53SEY lambda transition observed in the temperature range 323.2–323.5 K

TABLE 12.51.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57MCC/FIN2	234.2–344.5	37	0.20	0.461	2.58–2	0.09	–1.20–3	–1
63GUD/CAM	313.1–423.1	3	1.00#	2.381	7.20–1	2.38	3.63–1	–1
88SHI/OGA1	298.1	1	0.50#	0.188	2.62–2	0.09	2.62–2	1
89OHN/FUJ	298.1	1	0.50#	0.085	1.18–2	0.04	1.18–2	1
				Rejected data				
49PAR/HAT	(1.81–1, 0.70, 1.03–2, 1)			53SEY	(4.35–1, 1.41, 3.89–1, 6)			

TABLE 12.51.3. Parameters of regression polynomial

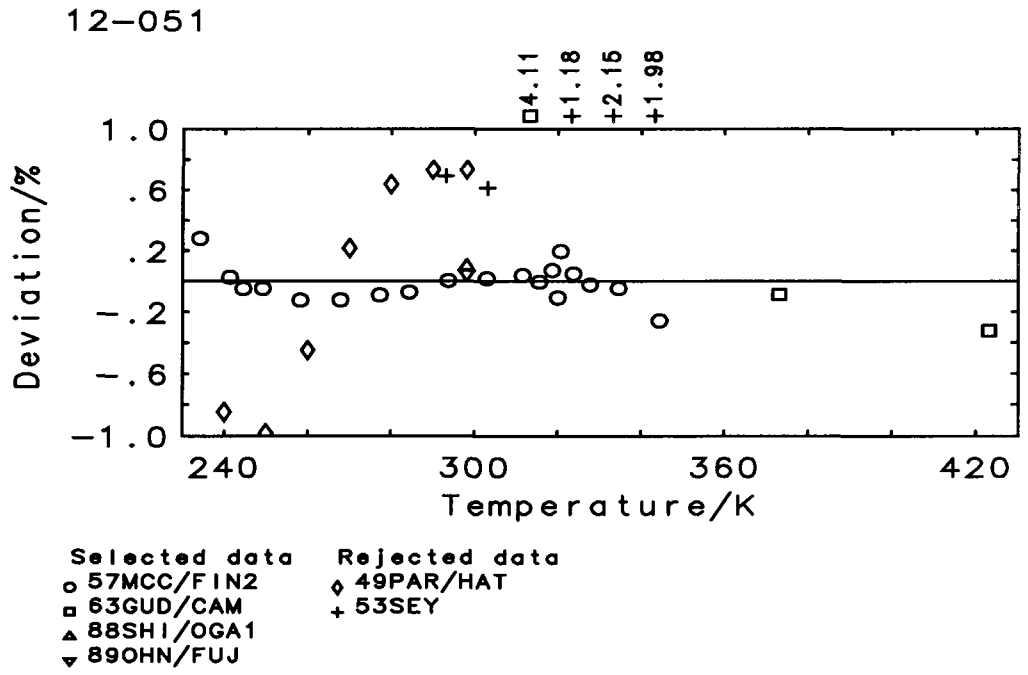
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	56	42	0.799	2.01–1	0.67	2.58–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
234.2–423.1		1.67823+1	6.02504–1	1.04870			III

TABLE 12.51.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1} g^{-1}$)	1.460	1.494	1.530	1.567	1.579	1.605	1.645
C ($J K^{-1} mol^{-1}$)	201.8	206.6	211.5	216.6	218.3	221.9	227.4
Temp. (K)	298.15	300	310	320	330	340	350
c ($J K^{-1} g^{-1}$)	1.678	1.686	1.728	1.771	1.816	1.862	1.909
C ($J K^{-1} mol^{-1}$)	232.0	233.0	238.9	244.9	251.0	257.4	263.9
Temp. (K)	360	370	380	390	400	410	420
c ($J K^{-1} g^{-1}$)	1.957	2.007	2.058	2.110	2.163	2.218	2.274
C ($J K^{-1} mol^{-1}$)	270.6	277.4	284.5	291.7	299.1	306.6	314.4

TABLE 12.51.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	56	42	1.106	1.98–1	0.66	–4.71–3	–29
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
234.2–423.1	702.30	–1.36540+1	3.29021	8.68558	1.41656+1		IV



Name: *trans*–Decahydronaphthalene
Formula: $C_{10}H_{18}$

CAS-RN: 493–02–7
Group No.: 12–052
Molar Mass: 138.25

TABLE 12.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49PAR/HAT	240.0–298.2	7S	0.70	98.9	melpt	C_p	BSIO	25PAR
53SEY	293.1–413.1	13S	nosp	not specified		C_p	BSAO	24WIL/DAN
57MCC/FIN2	248.8–344.3	13	0.20	99.98	melpt	C_{sat}	BSAO	47HUF
63GUD/CAM	313.1–423.1	3S	nosp	99.8	melpt	C_p	BDHT	63GUD/CAM
88SHI/OGA1	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA
89OHN/FUJ	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA

TABLE 12.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
53SEY	293.1–413.1	13	1.00#	0.918	2.97–1	0.92	1.86–1	6
57MCC/FIN2	248.8–344.3	13	0.20	0.626	3.76–2	0.13	–7.11–3	0
				Rejected data				
49PAR/HAT	(2.29–1, 0.87, 3.16–2, 0)			63GUD/CAM	(1.13, 3.74, 9.33–1, 2)			
88SHI/OGA1	(1.02–1, 0.37, 1.02–1, 1)			89OHN/FUJ	(1.02–1, 0.37, 1.02–1, 1)			

TABLE 12.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	38	26	0.836	2.25–1	0.70	8.95–2	6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
248.8–413.1		1.68061+1	4.81994–2	1.18237			IV

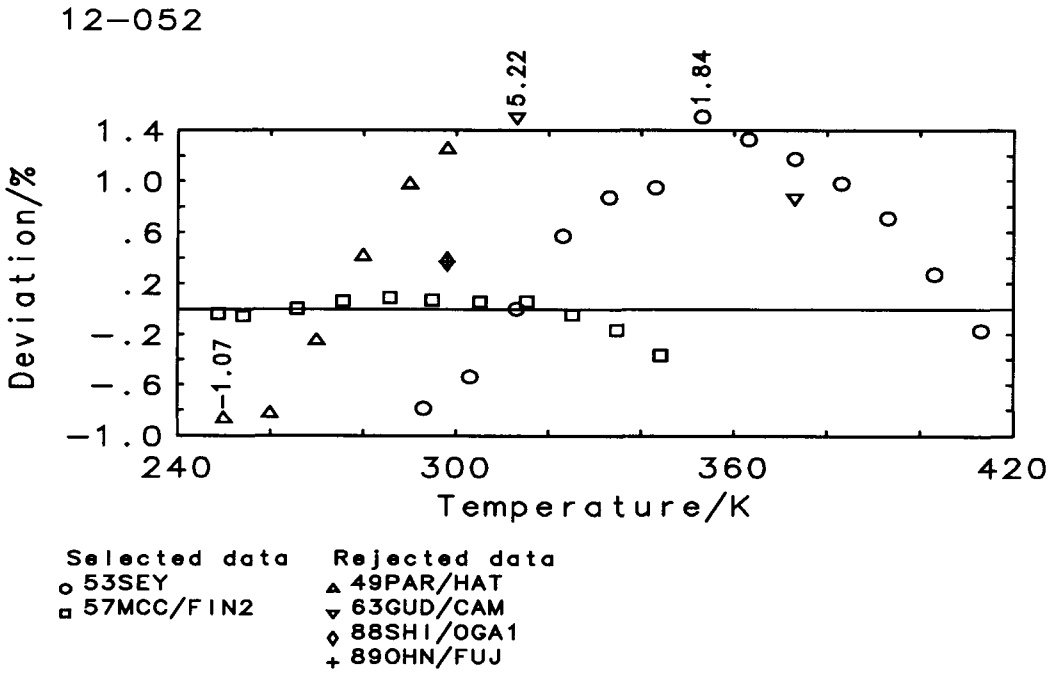
TABLE 12.52.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c ($J K^{-1} g^{-1}$)	1.462	1.499	1.537	1.549	1.576	1.617	1.651
C ($J K^{-1} mol^{-1}$)	202.2	207.2	212.5	214.2	217.9	223.6	228.3
Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	1.659	1.703	1.748	1.795	1.843	1.892	1.943
C ($J K^{-1} mol^{-1}$)	229.4	235.5	241.7	248.1	254.7	261.6	268.6
Temp. (K)	370	380	390	400	410		
c ($J K^{-1} g^{-1}$)	1.995	2.049	2.104	2.160	2.218		
C ($J K^{-1} mol^{-1}$)	275.8	283.2	290.8	298.6	306.6		

TABLE 12.52.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	38	26	2.017	1.40–1	0.47	1.75–2	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
248.8–413.1	687.10	1.90456+3	2.02414+2	–1.84462+2	1.77417+3	3.51300+2	1.24819+3	IV



Name: Octahydromethyl–1*H*–indene
Formula: $C_{10}H_{18}$

CAS–RN: unknown
Group No.: 12–053
Molar Mass: 138.25

TABLE 12.53.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–423.1	3	nosp	95.9	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	3.82–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–423.1		5.33793+1	–1.68620+1	3.18347			V

TABLE 12.53.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.91	1.93	1.95	1.98	2.01	2.04	2.08
C_p ($J K^{-1} mol^{-1}$)	264	266	269	273	277	282	287
Temp. (K)	380	390	400	410	420		
c_p ($J K^{-1} g^{-1}$)	2.12	2.17	2.22	2.27	2.33		
C_p ($J K^{-1} mol^{-1}$)	293	300	307	314	322		

Name: 2,6,6–Trimethylbicyclo[3.1.1]heptane
Formula: $C_{10}H_{18}$

CAS-RN: 473–55–2
Group No.: 12–054
Molar Mass: 138.25

TABLE 12.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	98.	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–423.1	3	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.54.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
62GOL/BEL	310.9–422.0	3	1.00#	0.060	1.86–2	0.06	1.28–2	2
63GUD/CAM	313.1–423.1	3	1.00#	0.062	1.91–2	0.06	–1.27–2	–1

TABLE 12.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.086	2.66–2	0.09	2.67–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–423.1		4.70112+1	−1.65904+1	3.35032			IV

TABLE 12.54.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.671	1.698	1.729	1.764	1.803	1.847	1.894
C_p (J K^{-1}mol^{-1})	231.0	234.7	239.0	243.9	249.3	255.3	261.8
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	1.945	2.001	2.060	2.123	2.191		
C_p (J K^{-1}mol^{-1})	268.9	276.6	284.8	293.6	302.9		

Name: Butylcyclohexane
Formula: $C_{10}H_{20}$

CAS-RN: 1678–93–9
Group No.: 12–055
Molar Mass: 140.27

TABLE 12.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65FIN/MES	207.5–365.4	21	0.20	99.97	melpt	C_{sat}	BSAO	47HUF

TABLE 12.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	21	21	0.096	5.99–3	0.02	9.08–7	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
207.5–365.4		3.18295+1	−1.06364+1	5.08397	−4.79809−1		II

TABLE 12.55.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.628	1.655	1.685	1.716	1.750	1.785	1.821
C_{sat} (J K^{-1}mol^{-1})	228.4	232.2	236.3	240.7	245.4	250.3	255.5
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.833	1.860	1.899	1.932	1.940	1.981	2.023
C_{sat} (J K^{-1}mol^{-1})	257.2	260.9	266.4	271.0	272.1	277.9	283.8
Temp. (K)	330	340	350	360	370		
c_{sat} (J K^{-1}g^{-1})	2.066	2.109	2.152	2.196	2.239		
C_{sat} (J K^{-1}mol^{-1})	289.8	295.8	301.9	308.0	314.0		

TABLE 12.55.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	21	21	1.004	6.44-2	0.20	2.16-4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
207.5-365.4	648.40	-1.14068+1	3.89369	1.44810+1	8.35427		II

Name: Diethylcyclohexane (unspecified isomer)
Formula: $C_{10}H_{20}$

CAS-RN: 1331-43-7
Group No.: 12-056
Molar Mass: 140.27

TABLE 12.56.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL	N	310.9-422.0	3	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1-423.1	3	nosp	not specified		C_p	BDHT	63GUD/CAM

62GOL/BEL mixture of isomers
63GUD/CAM sample contained 95 mol.% of major component (not specified)

TABLE 12.56.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
62GOL/BEL	310.9-422.0	3	1.00#	1.753	6.60-1	1.75	1.46-1	1
63GUD/CAM	313.1-423.1	3	1.00#	0.452	1.77-1	0.45	-1.17-1	-1

TABLE 12.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	1.568	5.91-1	1.57	1.43-2	0
Temp. range K		A_1	A_2				Level of uncertainty
310.9-423.1		6.80683	7.86799				V

TABLE 12.56.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.85	1.90	1.94	1.99	2.04	2.08	2.13
C_p (J K^{-1}mol^{-1})	259	266	272	279	286	292	299
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.18	2.22	2.27	2.32	2.36		
C_p (J K^{-1}mol^{-1})	305	312	318	325	331		

Name: 1,4–Diethylcyclohexane
Formula: $C_{10}H_{20}$

CAS-RN: 1679–00–1
Group No.: 12–057
Molar Mass: 140.27

TABLE 12.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	N	313.1–423.1	3	nosp	99.95	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	99.97	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (30 % *cis* and 70 % *trans*)
63GUD/CAM mixture of isomers (80 % *cis*)

TABLE 12.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
63GUD/CAM	313.1–423.1	3	1.00#	1.138	3.83–1	1.14	1.03–1	1
63GUD/CAM	313.1–423.1	3	1.00#	1.138	3.82–1	1.14	–8.54–2	–1

TABLE 12.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.610	5.41–1	1.61	8.69–3	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
313.1–423.1	6.28796+1	–2.12034+1	3.60397	IV

TABLE 12.57.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.884	1.893	1.906	1.923	1.945	1.971	2.001
C_p (J K^{-1}mol^{-1})	264.3	265.5	267.4	269.8	272.9	276.5	280.7
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.036	2.075	2.118	2.165	2.217		
C_p (J K^{-1}mol^{-1})	285.6	291.0	297.1	303.7	311.0		

Name: (1,1–Dimethylethyl)cyclohexane
Formula: $C_{10}H_{20}$

CAS-RN: 3178–22–1
Group No.: 12–058
Molar Mass: 140.27

TABLE 12.58.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–423.1	3	nosp	99.5	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.58.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.595	2.28–1	0.60	2.11–3	1
Temp. range K		A_1	A_2				Level of uncertainty
313.1–423.1		1.42431	9.69204				IV

TABLE 12.58.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.923	1.980	2.038	2.095	2.153	2.210	2.268
C_p (J K^{-1}mol^{-1})	269.7	277.8	285.8	293.9	301.9	310.0	318.1
Temp. (K)	390	400	410	420			
c_p (J K^{-1}g^{-1})	2.325	2.382	2.440	2.497			
C_p (J K^{-1}mol^{-1})	326.1	334.2	342.2	350.3			

Name: Decahydro–1–methylnaphthalene
Formula: $C_{11}H_{20}$

CAS-RN: 2958–75–0
Group No.: 12–059
Molar Mass: 152.28

TABLE 12.59.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL		310.9–422.0	3	nosp	98.5	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	98.5	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 27.2 % *cis*– and 71.3 % *trans*–isomers

TABLE 12.59.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.298	1.01–1	0.30	9.24–2	3
63GUD/CAM	313.1–423.1	3	1.00#	1.192	4.44–1	1.19	–8.43–2	–1

TABLE 12.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.064	3.95–1	1.06	4.08–3	2
Temp. range K		A_1	A_2				Level of uncertainty
310.9–423.1		6.18535	8.36547				IV

TABLE 12.59.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.754	1.799	1.845	1.891	1.936	1.982	2.028
C_p (J K^{-1}mol^{-1})	267.0	274.0	281.0	287.9	294.9	301.8	308.8
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.073	2.119	2.165	2.210	2.256		
C_p (J K^{-1}mol^{-1})	315.7	322.7	329.6	336.6	343.6		

Name: Decahydro–2–methylnaphthalene
Formula: $C_{11}H_{20}$

CAS-RN: 2958–76–1
Group No.: 12–060
Molar Mass: 152.28

TABLE 12.60.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL		310.9–422.0	3	nosp	99.5	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	99.5	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 61.6 % *cis*– and 37.9 % *trans*–isomers

TABLE 12.60.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.288	9.35–2	0.29	–8.33–2	–3
63GUD/CAM	313.1–423.1	3	1.00#	1.324	4.81–1	1.32	1.00–1	1

TABLE 12.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.174	4.24–1	1.17	8.48–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
310.9–423.1		2.40572	9.05443				V

TABLE 12.60.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.66	1.71	1.76	1.81	1.86	1.91	1.96
C_p (J K^{-1}mol^{-1})	253	261	268	276	283	291	299
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.01	2.06	2.11	2.16	2.21		
C_p (J K^{-1}mol^{-1})	306	314	321	329	336		

Name: Ethyloctahydro–1*H*–indene
Formula: $C_{11}H_{20}$

CAS-RN: 95098–51–4
Group No.: 12–061
Molar Mass: 152.28

TABLE 12.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.4	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–423.1	3	nosp	99.4	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.61.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.151	5.60–2	0.15	–1.32–2	–1
63GUD/CAM	313.1–423.1	3	1.00#	0.153	6.06–2	0.15	1.30–2	0

TABLE 12.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.186	7.15–2	0.19	–1.37–4	–1

Temp. range K	A_1	A_2	Level of uncertainty
310.9–423.1	1.01602+1	7.64425	IV

TABLE 12.61.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.849	1.890	1.932	1.974	2.016	2.057	2.099
C_p ($J K^{-1} mol^{-1}$)	281.5	287.9	294.2	300.6	306.9	313.3	319.6
Temp. (K)	380	390	400	410	420		
c_p ($J K^{-1} g^{-1}$)	2.141	2.183	2.224	2.266	2.308		
C_p ($J K^{-1} mol^{-1}$)	326.0	332.4	338.7	345.1	351.4		

Name: Decahydrodimethanonaphthalene
Formula: $C_{12}H_{18}$

CAS–RN: unknown
Group No.: 12–062
Molar Mass: 162.27

TABLE 12.62.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–423.1	3	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	2.54–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–423.1		−4.78160+1	3.94169+1	−4.35526			V

TABLE 12.62.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.67	1.73	1.78	1.84	1.89	1.93	1.97
C_p (J K^{-1}mol^{-1})	270	280	290	298	306	313	319
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.00	2.03	2.06	2.08	2.10		
C_p (J K^{-1}mol^{-1})	325	330	334	337	340		

Name: 1,3–Dimethyltricyclo[3.3.1.1^{3,7}]decane
Formula: $C_{12}H_{20}$

CAS-RN: 702–79–4
Group No.: 12–063
Molar Mass: 164.29

TABLE 12.63.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77STE/WAT	N	298.15	2.160	nosp	not specified		C_p	not specified	

77STE/WAT unspecified DSC calorimeter was used

Name: Tricyclo[6.2.1.1^{3,6}]dodecane
Formula: $C_{12}H_{20}$

CAS-RN: 281–84–5
Group No.: 12–064
Molar Mass: 164.29

TABLE 12.64.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL	N	310.9–422.0	3	nosp	98.5	chrom	C_p	BDHT	63GUD/CAM

62GOL/BEL probably an error in the name of substance; identified as Tetracyclo[6.2.1.1^{3,6}]dodecane by the authors

TABLE 12.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
310.9–422.0		1.00505+1	7.58954				V

TABLE 12.64.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.70	1.74	1.78	1.81	1.85	1.89	1.93
C_p ($J K^{-1} mol^{-1}$)	279	285	292	298	304	311	317
Temp. (K)	380	390	400	410	420		
c_p ($J K^{-1} g^{-1}$)	1.97	2.01	2.05	2.08	2.12		
C_p ($J K^{-1} mol^{-1}$)	323	330	336	342	349		

Name: 1,1'–Bicyclohexyl
Formula: $C_{12}H_{22}$

CAS-RN: 92–51–3
Group No.: 12–065
Molar Mass: 166.31

TABLE 12.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57PIL	276.9	1	nosp	99.9985	melpt	C_p	BSAO	57PIL
62GOL/BEL	310.9–422.0	3S	nosp	99.2	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	99.2	chrom	C_p	BDHT	63GUD/CAM
83ORO/MRA	279.1–470.0	47S	1.00	99.9	chrom	C_p	BDHT	69PER/COM

TABLE 12.65.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57PIL	276.9	1	0.50#	0.433	6.96–2	0.22	6.96–2	1
83ORO/MRA	279.1–470.0	47	1.00	0.774	2.84–1	0.77	–7.60–4	–7
				Rejected data				
62GOL/BEL	(1.01, 2.63, –3.17–1, –1)			63GUD/CAM	(9.54–1, 2.45, –3.72–1, –1)			

TABLE 12.65.3. Parameters of regression polynomial

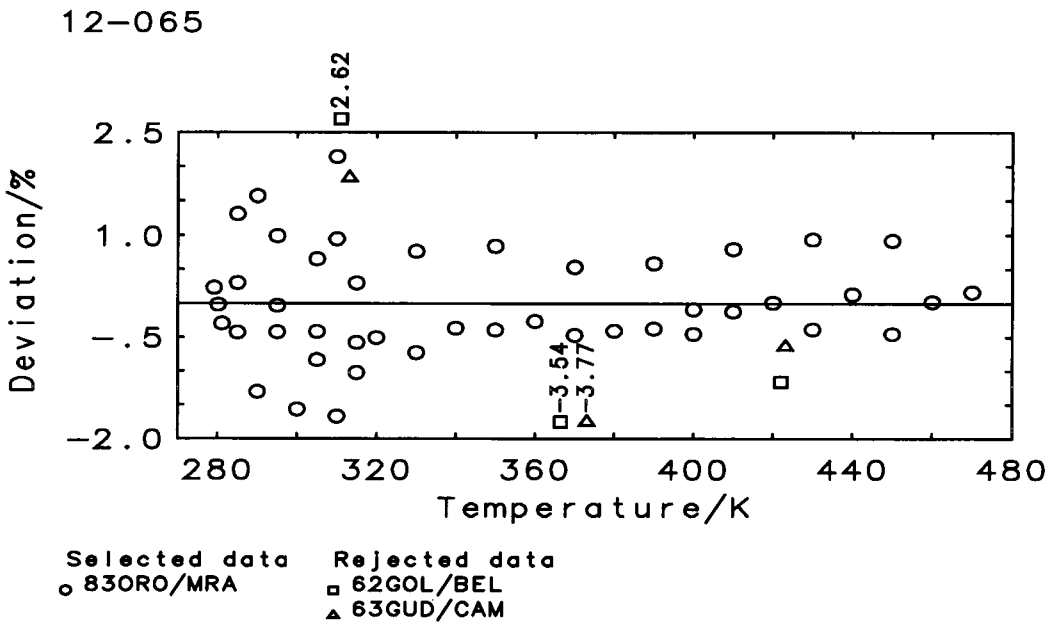
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	55	48	0.785	2.87–1	0.78	7.07–4	–6
Temp. range K		A_1	A_2				Level of uncertainty
276.9–470.0		6.73499	9.15668				IV

TABLE 12.65.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.619	1.664	1.702	1.710	1.756	1.802	1.847
C_p (J K^{-1}mol^{-1})	269.2	276.8	283.0	284.4	292.0	299.6	307.2
Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	1.893	1.939	1.985	2.031	2.076	2.122	2.168
C_p (J K^{-1}mol^{-1})	314.9	322.5	330.1	337.7	345.3	352.9	360.5
Temp. (K)	410	420	430	440	450	460	470
c_p (J K^{-1}g^{-1})	2.214	2.259	2.305	2.351	2.397	2.443	2.488
C_p (J K^{-1}mol^{-1})	368.1	375.8	383.4	391.0	398.6	406.2	413.8

TABLE 12.65.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	55	48	0.784	2.87–1	0.78	2.67–3	–12
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
276.9–470.0	899.00	–8.87719	2.95407–1	7.89791	6.66915+1		IV



Name: Decahydrodimethylnaphthalene
Formula: $C_{12}H_{22}$

CAS-RN: 28777–88–0
Group No.: 12–066
Molar Mass: 166.31

TABLE 12.66.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	N	313.1–483.1	4	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 37.3 mol.% of major component (not specified)

TABLE 12.66.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	4.737	2.07	4.74	5.53–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		7.61407+1	–2.77146+1	4.83646			V

TABLE 12.66.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	1.84	1.85	1.87	1.89	1.92	1.95	1.99
C_p ($J K^{-1}mol^{-1}$)	305	307	311	314	319	325	331
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1}g^{-1}$)	2.03	2.08	2.13	2.19	2.25	2.32	2.39
C_p ($J K^{-1}mol^{-1}$)	338	346	355	364	375	386	398
Temp. (K)	450	460	470	480			
c_p ($J K^{-1}g^{-1}$)	2.47	2.55	2.64	2.73			
C_p ($J K^{-1}mol^{-1}$)	410	424	438	453			

Name: Ethyldecahydronaphthalene
Formula: $C_{12}H_{22}$

CAS-RN: 25551–49–9
Group No.: 12–067
Molar Mass: 166.31

TABLE 12.67.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	N	313.1–483.1	4	nosp	98.7	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 40.2 mol.% of major component (not specified)

TABLE 12.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	3.342	1.48	3.34	2.78–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		5.03128+1	–1.48325+1	3.27849			VI

TABLE 12.67.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.79	1.82	1.85	1.89	1.93	1.97	2.02
C_p (J K^{-1}mol^{-1})	298	303	308	314	321	328	335
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.06	2.12	2.17	2.23	2.29	2.36	2.43
C_p (J K^{-1}mol^{-1})	343	352	361	371	381	392	403
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.50	2.57	2.65	2.73			
C_p (J K^{-1}mol^{-1})	415	428	441	454			

Name: 1–Ethyldecahydronaphthalene
Formula: $C_{12}H_{22}$

CAS-RN: 1008–17–9
Group No.: 12–068
Molar Mass: 166.31

TABLE 12.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.2	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM N	313.1–423.1	3	nosp	99.2	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (31.4 % *cis* and 67.8 % *trans*)

TABLE 12.68.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.058	2.56–2	0.06	9.30–3	1
63GUD/CAM	313.1–423.1	3	1.00#	0.363	1.51–1	0.36	–7.28–3	1

TABLE 12.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.319	1.32–1	0.32	1.01–3	2
Temp. range K		A_1	A_2				Level of uncertainty
310.9–423.1		1.15152+1	8.02962				IV

TABLE 12.68.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.820	1.860	1.900	1.941	1.981	2.021	2.061
C_p (J K^{-1}mol^{-1})	302.7	309.4	316.1	322.7	329.4	336.1	342.8
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.101	2.141	2.181	2.222	2.262		
C_p (J K^{-1}mol^{-1})	349.4	356.1	362.8	369.5	376.1		

Name: 2–Ethyldecahydronaphthalene
Formula: $C_{12}H_{22}$

CAS-RN: 1618–23–1
Group No.: 12–069
Molar Mass: 166.31

TABLE 12.69.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL		310.9–422.0	3	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–423.1	3	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 31.7 % *cis*– and 68.1 % *trans*–isomers

TABLE 12.69.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.056	2.25–2	0.06	–8.76–3	0
63GUD/CAM	313.1–423.1	3	1.00#	0.214	8.68–2	0.21	9.84–3	1

TABLE 12.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.192	7.77–2	0.19	5.42–4	1
Temp. range K		A_1	A_2				Level of uncertainty
310.9–423.1		8.01315	8.64761				IV

TABLE 12.69.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.741	1.784	1.827	1.871	1.914	1.957	2.000
C_p (J K^{-1}mol^{-1})	289.5	296.7	303.9	311.1	318.3	325.5	332.7
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.044	2.087	2.130	2.173	2.216		
C_p (J K^{-1}mol^{-1})	339.8	347.0	354.2	361.4	368.6		

Name: Octahydro(1–methylethyl)–1*H*–indene
Formula: $C_{12}H_{22}$

CAS-RN: 88889–26–3
Group No.: 12–070
Molar Mass: 166.31

TABLE 12.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	93.5	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–423.1	3	nosp	93.5	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.70.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
62GOL/BEL	310.9–422.0	3	1.00#	0.644	2.76–1	0.64	4.84–3	–1
63GUD/CAM	313.1–423.1	3	1.00#	0.637	2.78–1	0.64	1.12–3	–1

TABLE 12.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.785	3.39–1	0.78	2.98–3	–2

Temp. range K	A_1	A_2	Level of uncertainty
310.9–423.1	2.38940+1	5.13264	V

TABLE 12.70.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.99	2.02	2.04	2.07	2.09	2.12	2.14
C_p ($J K^{-1} mol^{-1}$)	331	335	339	344	348	352	357
Temp. (K)	380	390	400	410	420		
c_p ($J K^{-1} g^{-1}$)	2.17	2.20	2.22	2.25	2.27		
C_p ($J K^{-1} mol^{-1}$)	361	365	369	374	378		

Name: 1,3,5–Trimethyltricyclo[3.3.1.$1^{3,7}$]decane
Formula: $C_{13}H_{22}$

CAS-RN: 707–35–7
Group No.: 12–071
Molar Mass: 178.32

TABLE 12.71.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77STE/WAT	N	298.15	1.920	nosp	99.95	melpt	C_p	not specified	

77STE/WAT unspecified DSC calorimeter was used

Name: Decahydro(1–methylethyl)naphthalene
Formula: $C_{13}H_{24}$

CAS-RN: 27193–29–9
Group No.: 12–072
Molar Mass: 180.33

TABLE 12.72.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	N	373.1–483.1	3	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 52.2 mol.% of major component (not specified)

TABLE 12.72.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	7.63–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
373.1–483.1		1.50315+2	–5.92345+1	8.30490			V

TABLE 12.72.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.07	2.08	2.10	2.13	2.17	2.21	2.27
C_p (J K^{-1}mol^{-1})	373	375	379	385	391	399	409
Temp. (K)	440	450	460	470	480		
c_p (J K^{-1}g^{-1})	2.33	2.39	2.47	2.55	2.64		
C_p (J K^{-1}mol^{-1})	420	432	445	460	477		

Name: Decahydro–1–(1–methylethyl)naphthalene
Formula: $C_{13}H_{24}$

CAS-RN: 1010–74–8
Group No.: 12–073
Molar Mass: 180.33

TABLE 12.73.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL		310.9–422.0	3	nosp	98.9	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	312.0–483.1	4	nosp	98.9	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (22.3 % *cis* and 76.6 % *trans*)

TABLE 12.73.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
62GOL/BEL	310.9–422.0	3	1.00#	0.087	3.74–2	0.09	6.70–4	0
63GUD/CAM	312.0–483.1	4	1.00#	0.310	1.35–1	0.31	1.11–3	0

TABLE 12.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.286	1.24–1	0.29	9.24–4	0
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		6.83533	1.00451+1				IV

TABLE 12.73.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.751	1.797	1.844	1.890	1.936	1.982	2.029
C_p (J K^{-1}mol^{-1})	315.7	324.1	332.4	340.8	349.2	357.5	365.9
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.075	2.121	2.168	2.214	2.260	2.307	2.353
C_p (J K^{-1}mol^{-1})	374.2	382.6	390.9	399.3	407.6	416.0	424.3
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.399	2.446	2.492	2.538			
C_p (J K^{-1}mol^{-1})	432.7	441.0	449.4	457.7			

Name: Decahydro–1–propylnaphthalene
Formula: $C_{13}H_{24}$

CAS-RN: 91972–45–1
Group No.: 12–074
Molar Mass: 180.33

TABLE 12.74.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL		310.9–422.0	3S	nosp	98.2	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–483.1	4	nosp	98.2	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (*cis* 32.0 % and *trans* 66.2 %)

TABLE 12.74.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.543	2.50–1	0.54	3.58–2	–1
63GUD/CAM	313.1–483.1	3	1.00#	0.332	1.75–1	0.33	–3.11–2	–1

TABLE 12.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.636	3.05–1	0.64	2.33–3	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–483.1		3.60317+1	–4.18632	1.80306			V

TABLE 12.74.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.86	1.89	1.93	1.97	2.00	2.04	2.09
C_p (J K^{-1}mol^{-1})	336	342	348	355	361	369	376
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.13	2.17	2.22	2.27	2.32	2.37	2.42
C_p (J K^{-1}mol^{-1})	384	392	400	409	418	427	437
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.48	2.53	2.59	2.65			
C_p (J K^{-1}mol^{-1})	447	457	467	478			

Name: 2–Methyl–1,1'–bicyclohexyl
Formula: $C_{13}H_{24}$

CAS–RN: unknown
Group No.: 12–075
Molar Mass: 180.33

TABLE 12.75.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	98.8	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.75.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.604	7.38–1	1.60	1.90–2	2
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		2.16555	1.19129+1				V

TABLE 12.75.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	1.80	1.86	1.91	1.97	2.02	2.08	2.13
C_p ($J\,K^{-1}mol^{-1}$)	325	335	345	355	365	375	384
Temp. (K)	380	390	400	410	420	430	440
c_p ($J\,K^{-1}g^{-1}$)	2.19	2.24	2.30	2.35	2.41	2.46	2.52
C_p ($J\,K^{-1}mol^{-1}$)	394	404	414	424	434	444	454
Temp. (K)	450	460	470	480			
c_p ($J\,K^{-1}g^{-1}$)	2.57	2.63	2.68	2.74			
C_p ($J\,K^{-1}mol^{-1}$)	464	474	484	493			

Name: 1,1'–Methylenebiscyclohexane
Formula: $C_{13}H_{24}$

CAS-RN: 3178–23–2
Group No.: 12–076
Molar Mass: 180.33

TABLE 12.76.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3S	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	100.0	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.76.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
62GOL/BEL	310.9–422.0	3	1.00#	0.607	2.90–1	0.61	1.92–1	1
63GUD/CAM	373.1–483.1	3	1.00#	0.707	3.63–1	0.71	–1.82–1	–1

TABLE 12.76.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.932	4.65–1	0.93	4.73–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–483.1		4.89274+1	–9.19220	2.32660			IV

TABLE 12.76.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.973	1.998	2.025	2.055	2.087	2.120	2.156
C_p (J K^{-1}mol^{-1})	355.8	360.3	365.3	370.6	376.3	382.4	388.8
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.194	2.235	2.277	2.321	2.368	2.417	2.468
C_p (J K^{-1}mol^{-1})	395.7	403.0	410.6	418.6	427.0	435.8	445.0
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.521	2.576	2.634	2.693			
C_p (J K^{-1}mol^{-1})	454.6	464.6	474.9	485.6			

Name: Heptylcyclohexane
Formula: $C_{13}H_{26}$

CAS-RN: 5617–41–4
Group No.: 12–077
Molar Mass: 182.35

TABLE 12.77.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49PAR/MOO	240.0–300.0	7S	1.00	97.1	melpt	C_p	BSIO	25PAR

TABLE 12.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.192	7.86–2	0.19	2.93–4	0
Temp. range K		A_1	A_2				Level of uncertainty
240.0–300.0		2.02178+1	7.85827				V

TABLE 12.77.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.78	1.82	1.85	1.89	1.90	1.93	1.96
C_p (J K^{-1}mol^{-1})	325	331	338	345	347	351	358
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.99	2.00					
C_p (J K^{-1}mol^{-1})	363	364					

Name: Decahydro–3,5,1,7–[1,2,3,4]butanetetraylnaphthalene
Formula: $C_{14}H_{20}$

CAS-RN: 2292–79–7
Group No.: 12–078
Molar Mass: 188.31

TABLE 12.78.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78SPI/AND	519.2–537.1	7	nosp	99.91	melpt	C_p	BSAO	68WES/WES

TABLE 12.78.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.080	1.72–2	0.03	8.72–6	0
Temp. range K		A_1	A_2				Level of uncertainty
519.2–537.1		6.49683	8.92994				III

TABLE 12.78.4. Recommended values of heat capacities

Temp. (K)	520	530	540
c_p ($J\,K^{-1}g^{-1}$)	2.337	2.377	2.416
C_p ($J\,K^{-1}mol^{-1}$)	440.1	447.5	455.0

Name: Dodecahydro–9–methylfluorene
Formula: $C_{14}H_{24}$

CAS-RN: 92431–75–9
Group No.: 12–079
Molar Mass: 192.34

TABLE 12.79.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.79.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.319	6.12–1	1.32	3.78–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		4.49872	1.10730+1				V

TABLE 12.79.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.68	1.73	1.77	1.82	1.87	1.92	1.97
C_p (J K^{-1}mol^{-1})	323	332	341	350	360	369	378
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.01	2.06	2.11	2.16	2.20	2.25	2.30
C_p (J K^{-1}mol^{-1})	387	396	406	415	424	433	442
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.35	2.40	2.44	2.49			
C_p (J K^{-1}mol^{-1})	452	461	470	479			

Name: Tetradecahydrophenanthrene
Formula: $C_{14}H_{24}$

CAS-RN: 5743–97–5
Group No.: 12–080
Molar Mass: 192.34

TABLE 12.80.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.056	5.44–1	1.06	1.50–3	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		9.60103	9.63400				V

TABLE 12.80.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.71	1.75	1.79	1.83	1.87	1.91	1.96
C_p (J K^{-1}mol^{-1})	328	336	344	352	360	368	376
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.00	2.04	2.08	2.12	2.16	2.21	2.25
C_p (J K^{-1}mol^{-1})	384	392	400	408	416	424	432
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.29	2.33	2.37	2.41			
C_p (J K^{-1}mol^{-1})	440	448	456	464			

Name: (4aα,4bα,8aα,10aβ)–Tetradecahydrophenanthrene
Formula: $C_{14}H_{24}$

CAS-RN: 27425–35–0
Group No.: 12–081
Molar Mass: 192.34

TABLE 12.81.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82NUZ	283.0–403.0	14S	nosp	not specified		C_p	BDHT	73PER/COM

TABLE 12.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.920	6.20–1	1.38	1.36–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
283.0–403.0		5.19497+1	–1.44099+1	3.64063			V

TABLE 12.81.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.76	1.79	1.79	1.83	1.86	1.90	1.95
C_p (J K^{-1}mol^{-1})	339	344	345	351	359	366	375
Temp. (K)	350	360	370	380	390	400	
c_p (J K^{-1}g^{-1})	1.99	2.04	2.10	2.15	2.21	2.27	
C_p (J K^{-1}mol^{-1})	383	393	403	414	425	437	

Name: (4aα,4bβ,8aα,10aα)–Tetradecahydrophenanthrene
Formula: $C_{14}H_{24}$

CAS-RN: 27389–73–7
Group No.: 12–082
Molar Mass: 192.34

TABLE 12.82.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82NUZ	323.0–403.0	9S	nosp	not specified		C_p	BDHT	73PER/COM

TABLE 12.82.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	1.822	1.04	2.73	4.67–2	5
Temp. range K		A_1	A_2				Level of uncertainty
323.0–403.0		–4.44900+1	2.43424+1				V

TABLE 12.82.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.44	1.55	1.65	1.76	1.86	1.97	2.08
C_p (J K^{-1}mol^{-1})	278	298	318	338	359	379	399
Temp. (K)	390	400					
c_p (J K^{-1}g^{-1})	2.18	2.29					
C_p (J K^{-1}mol^{-1})	419	440					

Name: (4aα,4bβ,8aα,10aβ)–Tetradecahydrophenanthrene
Formula: $C_{14}H_{24}$

CAS-RN: 2108–89–6
Group No.: 12–083
Molar Mass: 192.34

TABLE 12.83.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
82NUZ	293.0–403.0	13S	nosp	not specified		C_p	BDHT	73PER/COM

TABLE 12.83.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	2.151	1.38	3.23	6.81–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
293.0–403.0		–2.35193+1	1.93147+1				VI

TABLE 12.83.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.40	1.47	1.49	1.57	1.66	1.74	1.82
C_p (J K^{-1}mol^{-1})	270	283	286	302	318	334	350
Temp. (K)	350	360	370	380	390	400	
c_p (J K^{-1}g^{-1})	1.91	1.99	2.07	2.16	2.24	2.32	
C_p (J K^{-1}mol^{-1})	367	383	399	415	431	447	

Name: 1–Butyldecahydronaphthalene
Formula: $C_{14}H_{26}$

CAS-RN: 92369–80–7
Group No.: 12–084
Molar Mass: 194.36

TABLE 12.84.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL		310.9–422.0	3	nosp	99.5	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–483.1	4	nosp	99.5	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (25.2 % *cis* and 74.3 % *trans*)

TABLE 12.84.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	3.258	1.63	3.26	−1.20	−1
63GUD/CAM	313.1–483.1	4	1.00#	2.000	1.13	2.00	1.04	4

TABLE 12.84.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	3.094	1.61	3.09	8.01–2	3
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		1.16844+1	9.96577				VI

TABLE 12.84.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.82	1.86	1.91	1.95	1.99	2.03	2.08
C_p (J K^{-1}mol^{-1})	354	362	371	379	387	395	404
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.12	2.16	2.21	2.25	2.29	2.33	2.38
C_p (J K^{-1}mol^{-1})	412	420	429	437	445	453	462
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.42	2.46	2.50	2.55			
C_p (J K^{-1}mol^{-1})	470	478	487	495			

Name: 1-(Cyclohexylmethyl)-2-methylcyclohexane
Formula: $C_{14}H_{26}$

CAS-RN: 66826-96-8
Group No.: 12-085
Molar Mass: 194.36

TABLE 12.85.1. *Experimental heat capacities*

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.85.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	2.491	1.25	2.49	1.89–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		9.18962+1	−3.24988+1	5.45448			V

TABLE 12.85.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.86	1.87	1.88	1.90	1.92	1.95	1.98
C_p (J K^{-1}mol^{-1})	362	364	366	370	374	379	385
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.02	2.06	2.10	2.15	2.21	2.27	2.33
C_p (J K^{-1}mol^{-1})	392	400	409	419	429	441	453
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.40	2.47	2.55	2.63			
C_p (J K^{-1}mol^{-1})	466	481	496	512			

Name: Decahydro–1–(1–methylpropyl)naphthalene
Formula: $C_{14}H_{26}$

CAS-RN: 92369–82–9
Group No.: 12–086
Molar Mass: 194.36

TABLE 12.86.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL		310.9–422.0	3	nosp	98.3	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–483.1	4	nosp	98.3	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (37.4 % *cis* and 60.9 % *trans*)

TABLE 12.86.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.741	3.84–1	0.74	2.66–1	1
63GUD/CAM	313.1–483.1	4	1.00#	1.480	7.73–1	1.48	–1.71–1	0

TABLE 12.86.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	1.613	8.42–1	1.61	1.63–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–483.1		3.41286+1	–2.86511	1.76221			V

TABLE 12.86.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.80	1.84	1.88	1.91	1.95	2.00	2.04
C_p (J K^{-1}mol^{-1})	351	358	365	372	380	388	396
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.08	2.13	2.18	2.22	2.27	2.33	2.38
C_p (J K^{-1}mol^{-1})	405	414	423	432	442	452	463
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.43	2.49	2.55	2.61			
C_p (J K^{-1}mol^{-1})	473	484	495	507			

Name: Decahydro–1–(2–methylpropyl)naphthalene
Formula: $C_{14}H_{26}$

CAS-RN: 92369–83–0
Group No.: 12–087
Molar Mass: 194.36

TABLE 12.87.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	N	313.1–483.1	4	nosp	98.7	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM mixture of isomers (44.6 % *cis* and 54.1 % *trans*)

TABLE 12.87.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.966	9.85–1	1.97	1.16–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		7.49411+1	–2.34307+1	4.25354			V

TABLE 12.87.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.85	1.86	1.88	1.90	1.93	1.96	1.99
C_p (J K^{-1}mol^{-1})	359	362	365	370	374	380	386
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.02	2.06	2.11	2.16	2.21	2.26	2.32
C_p (J K^{-1}mol^{-1})	393	401	410	419	429	439	451
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.38	2.45	2.51	2.59			
C_p (J K^{-1}mol^{-1})	463	475	489	503			

Name: (1,1–Dimethylethyl)decahydronaphthalene
Formula: $C_{14}H_{26}$

CAS-RN: 27193–30–2
Group No.: 12–088
Molar Mass: 194.36

TABLE 12.88.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–423.1	3	nosp	99.4	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.88.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.402	1.97–1	0.40	–1.33–4	–1

Temp. range K	A_1	A_2	Level of uncertainty
313.1–423.1	1.13587+1	9.91416	V

TABLE 12.88.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.80	1.84	1.89	1.93	1.97	2.01	2.06
C_p (J K^{-1}mol^{-1})	350	358	366	375	383	391	399
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.10	2.14	2.18	2.22	2.27		
C_p (J K^{-1}mol^{-1})	408	416	424	432	441		

Name: 1,1'–(1,2–Ethanediyl)biscyclohexane
Formula: $C_{14}H_{26}$

CAS-RN: 3321–50–4
Group No.: 12–089
Molar Mass: 194.36

TABLE 12.89.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	99.7	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.89.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.527	2.76–1	0.53	1.18–3	0

Temp. range K	A_1	A_2	Level of uncertainty
313.1–483.1	1.33815+1	9.86702	IV

TABLE 12.89.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.881	1.923	1.965	2.008	2.050	2.092	2.134
C_p (J K^{-1}mol^{-1})	365.6	373.8	382.0	390.2	398.4	406.6	414.8
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.176	2.219	2.261	2.303	2.345	2.387	2.430
C_p (J K^{-1}mol^{-1})	423.0	431.2	439.4	447.6	455.8	464.0	472.2
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.472	2.514	2.556	2.599			
C_p (J K^{-1}mol^{-1})	480.4	488.6	496.8	505.0			

Name: 2–Ethyl–1,1'–bicyclohexyl
Formula: $C_{14}H_{26}$

CAS-RN: 66826–94–6
Group No.: 12–090
Molar Mass: 194.36

TABLE 12.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.90.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.066	3.55–2	0.07	3.81–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		3.64918+1	–3.24819	1.84457			IV

TABLE 12.90.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.889	1.924	1.962	2.001	2.041	2.084	2.127
C_p (J K^{-1}mol^{-1})	367.1	374.0	381.3	388.9	396.8	405.0	413.4
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.172	2.219	2.268	2.318	2.369	2.423	2.477
C_p (J K^{-1}mol^{-1})	422.2	431.4	440.8	450.5	460.5	470.9	481.5
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.534	2.592	2.651	2.712			
C_p (J K^{-1}mol^{-1})	492.4	503.7	515.3	527.1			

Name: 1,1'–Ethylidenebiscyclohexane
Formula: $C_{14}H_{26}$

CAS-RN: 2319–61–1
Group No.: 12–091
Molar Mass: 194.36

TABLE 12.91.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	99.	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.91.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.839	9.19–1	1.84	9.13–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		5.56176	1.17308+1				V

TABLE 12.91.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.79	1.84	1.89	1.94	1.99	2.04	2.09
C_p (J K^{-1}mol^{-1})	349	358	368	378	388	397	407
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.14	2.20	2.25	2.30	2.35	2.40	2.45
C_p (J K^{-1}mol^{-1})	417	427	436	446	456	466	475
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.50	2.55	2.60	2.65			
C_p (J K^{-1}mol^{-1})	485	495	505	514			

Name: 1,1':3',1''–Tercyclopentane
Formula: $C_{15}H_{26}$

CAS-RN: 6051–40–7
Group No.: 12–092
Molar Mass: 206.37

TABLE 12.92.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.92.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.167	6.14–1	1.17	7.20–3	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		1.31200+1	9.80976				V

TABLE 12.92.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.75	1.79	1.83	1.87	1.91	1.95	1.99
C_p (J K^{-1}mol^{-1})	362	370	378	386	395	403	411
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.03	2.07	2.11	2.15	2.19	2.23	2.27
C_p (J K^{-1}mol^{-1})	419	427	435	443	452	460	468
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.31	2.35	2.39	2.43			
C_p (J K^{-1}mol^{-1})	476	484	492	501			

Name: Cyclohexyl(ethylcyclohexyl)methane (unspecified isomer)
Formula: $C_{15}H_{28}$

CAS-RN: 97239-02-6
Group No.: 12-093
Molar Mass: 208.39

TABLE 12.93.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL		422.0	1	nosp	100.0	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–483.1	4	nosp	100.0	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 49.2 % of major component (not specified)

TABLE 12.93.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	422.0	1	1.00#	0.150	8.88–2	0.15	8.88–2	1
63GUD/CAM	313.1–483.1	4	1.00#	0.054	3.03–2	0.05	–2.22–2	–2

TABLE 12.93.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.131	7.61–2	0.13	4.88–5	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		3.81731+1	–1.52507	1.53372			V

TABLE 12.93.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.92	1.95	1.99	2.02	2.06	2.10	2.14
C_p ($J K^{-1} mol^{-1}$)	401	407	414	422	429	437	445
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.18	2.22	2.26	2.30	2.35	2.39	2.44
C_p ($J K^{-1} mol^{-1}$)	453	462	471	480	489	499	508
Temp. (K)	450	460	470	480			
c_p ($J K^{-1} g^{-1}$)	2.49	2.54	2.59	2.64			
C_p ($J K^{-1} mol^{-1}$)	519	529	539	550			

Name: 1-(Cyclohexylmethyl)-2-ethylcyclohexane
Formula: $C_{15}H_{28}$

CAS-RN: 66374-71-8
Group No.: 12-094
Molar Mass: 208.39

TABLE 12.94.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	99.8	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.94.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.296	1.65–1	0.30	-3.39–3	–1
63GUD/CAM	313.1–483.1	4	1.00#	0.256	1.54–1	0.26	4.79–3	0

TABLE 12.94.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.362	2.10–1	0.36	1.28–3	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–483.1		6.46970+1	–1.50303+1	3.26580			IV

TABLE 12.94.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.975	1.997	2.021	2.049	2.079	2.111	2.146
C_p (J K^{-1}mol^{-1})	411.5	416.1	421.2	426.9	433.2	439.9	447.3
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.184	2.224	2.267	2.313	2.361	2.412	2.465
C_p (J K^{-1}mol^{-1})	455.1	463.5	472.5	482.0	492.0	502.6	513.8
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.521	2.580	2.641	2.705			
C_p (J K^{-1}mol^{-1})	525.4	537.6	550.4	563.7			

Name: 1,2–Dicyclohexylpropane
Formula: $C_{15}H_{28}$

CAS-RN: 41851–34–7
Group No.: 12–095
Molar Mass: 208.39

TABLE 12.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	422.0	1	nosp	100.0	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	100.0	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.95.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	422.0	1	1.00#	0.041	2.47–2	0.04	–2.47–2	–1
63GUD/CAM	313.1–483.1	4	1.00#	0.604	3.43–1	0.60	1.10–2	0

TABLE 12.95.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.698	3.97–1	0.70	3.85–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		1.29566+1	1.11236+1				V

TABLE 12.95.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	1.89	1.94	1.98	2.03	2.07	2.11	2.16
C_p ($J K^{-1}mol^{-1}$)	394	404	413	422	431	441	450
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1}g^{-1}$)	2.20	2.25	2.29	2.34	2.38	2.43	2.47
C_p ($J K^{-1}mol^{-1}$)	459	468	478	487	496	505	515
Temp. (K)	450	460	470	480			
c_p ($J K^{-1}g^{-1}$)	2.51	2.56	2.60	2.65			
C_p ($J K^{-1}mol^{-1}$)	524	533	542	552			

Name: (1–Methylethyl)–1,1'–bicyclohexyl (unspecified isomer)
Formula: $C_{15}H_{28}$

CAS-RN: 31624–59–6
Group No.: 12–096
Molar Mass: 208.39

TABLE 12.96.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL	N	310.9–422.0	3	nosp	99.6	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	N	313.1–483.1	4	nosp	99.	chrom	C_p	BDHT	63GUD/CAM

62GOL/BEL isomer with n.m.t. 239.3 K
63GUD/CAM low boiling isomer

TABLE 12.96.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.125	7.33–2	0.13	4.67–2	1
63GUD/CAM	313.1–483.1	4	1.00#	0.280	1.58–1	0.28	–3.48–2	–2

TABLE 12.96.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.268	1.53–1	0.27	1.41–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		2.42297+1	8.36946				V

TABLE 12.96.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.00	2.04	2.07	2.10	2.14	2.17	2.20
C_p (J K^{-1}mol^{-1})	417	424	431	438	445	452	459
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.24	2.27	2.30	2.34	2.37	2.40	2.44
C_p (J K^{-1}mol^{-1})	466	473	480	487	494	501	508
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.47	2.50	2.54	2.57			
C_p (J K^{-1}mol^{-1})	515	522	529	535			

Name: Decylcyclopentane
Formula: $C_{15}H_{30}$

CAS-RN: 1795–21–7
Group No.: 12–097
Molar Mass: 210.40

TABLE 12.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65MES/TOD1	258.2–321.4	12	0.20	99.9	melpt	C_{sat}	BSAO	47HUF

TABLE 12.97.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.425	4.27–2	0 08	5.28–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
258.2–321.4		6.86653+1	–1.97027+1	4.64983			II

TABLE 12.97.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.931	1.951	1.958	1.974	2.001	2.025	2.031
C_{sat} (J K^{-1}mol^{-1})	406.3	410.4	411.9	415.3	421.0	426.2	427.4
Temp. (K)	310	320					
c_{sat} (J K^{-1}g^{-1})	2.066	2.104					
C_{sat} (J K^{-1}mol^{-1})	434.6	442.6					

TABLE 12.97.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.539	5.41–2	0.11	8.36–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
258.2–321.4	729.10	3.10354+2	1.45945+2	–9.99464+1	1.64994+2		II

Name: 1–Cyclohexyloctahydro–3–methyl–1*H*–indene
Formula: $C_{16}H_{28}$

CAS–RN: unknown
Group No.: 12–098
Molar Mass: 220.40

TABLE 12.98.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	99.3	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.98.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	2.305	1.38	2.31	3.55–2	0

Temp. range K	A_1	A_2	Level of uncertainty
313.1–483.1	1.43593+1	1.09394+1	V

TABLE 12.98.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.82	1.86	1.90	1.94	1.99	2.03	2.07
C_p (J K^{-1}mol^{-1})	401	410	420	429	438	447	456
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.11	2.15	2.19	2.23	2.27	2.32	2.36
C_p (J K^{-1}mol^{-1})	465	474	483	492	501	510	520
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.40	2.44	2.48	2.52			
C_p (J K^{-1}mol^{-1})	529	538	547	556			

Name: 2–Ethyltetradecahydrophenanthrene
Formula: $C_{16}H_{28}$

CAS-RN: 90591–84–7
Group No.: 12–099
Molar Mass: 220.40

TABLE 12.99.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.99.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	2.278	1.30	2.28	1.35–2	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
313.1–483.1	5.14849+1	–8.78911	2.47961	V

TABLE 12.99.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.81	1.84	1.87	1.90	1.93	1.96	2.00
C_p (J K^{-1}mol^{-1})	400	405	411	418	425	432	440
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.03	2.07	2.11	2.16	2.20	2.25	2.29
C_p (J K^{-1}mol^{-1})	448	457	466	475	485	495	506
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.34	2.40	2.45	2.51			
C_p (J K^{-1}mol^{-1})	517	528	540	552			

Name: 1,1'–(1–Methyl–1,3–propanediyl)biscyclohexane
Formula: $C_{16}H_{30}$

CAS-RN: 41851–35–8
Group No.: 12–100
Molar Mass: 222.41

TABLE 12.100.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	96.0	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.100.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.387	2.44–1	0.39	2.27–3	2
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		1.03655+1	1.20838+1				IV

TABLE 12.100.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.788	1.833	1.878	1.923	1.969	2.014	2.059
C_p (J K^{-1}mol^{-1})	397.6	407.7	417.7	427.8	437.8	447.9	457.9
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.104	2.149	2.194	2.240	2.285	2.330	2.375
C_p (J K^{-1}mol^{-1})	468.0	478.0	488.1	498.1	508.2	518.2	528.3
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.420	2.465	2.511	2.556			
C_p (J K^{-1}mol^{-1})	538.3	548.4	558.4	568.4			

Name: Cyclohexyl[(1–methylethyl)cyclohexyl]methane
Formula: $C_{16}H_{30}$

CAS-RN: 97676–41–0
Group No.: 12–101
Molar Mass: 222.41

TABLE 12.101.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	N	313.1–483.1	4	nosp	99.6	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 66.7 % of major component (not specified)

TABLE 12.101.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.820	5.27–1	0.82	6.05–3	2

Temp. range K	A_1	A_2	Level of uncertainty
313.1–483.1	1.69477+1	1.10552+1	V

TABLE 12.101.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.91	1.96	2.00	2.04	2.08	2.12	2.16
C_p (J K^{-1}mol^{-1})	426	435	444	453	463	472	481
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.20	2.25	2.29	2.33	2.37	2.41	2.45
C_p (J K^{-1}mol^{-1})	490	499	509	518	527	536	545
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.49	2.53	2.58	2.62			
C_p (J K^{-1}mol^{-1})	555	564	573	582			

Name: Decylcyclohexane
Formula: $C_{16}H_{32}$

CAS-RN: 1795–16–0
Group No.: 12–102
Molar Mass: 224.43

TABLE 12.102.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65FIN/MES	274.3–300.5	9	0.20	99.91	melpt	C_{sat}	BSAO	47HUF

TABLE 12.102.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.192	2.04–2	0.04	1.40–5	0
Temp. range K		A_1	A_2				Level of uncertainty
274.3–300.5		2.86344+1	8.63524				II

TABLE 12.102.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.957	1.989	2.015	2.021
C_{sat} (J K^{-1}mol^{-1})	439.1	446.3	452.1	453.5

Name: Cyclopentylbicyclohexyl (unspecified isomer)
Formula: $C_{17}H_{30}$

CAS-RN: 26447–22–3
Group No.: 12–103
Molar Mass: 234.43

TABLE 12.103.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62GOL/BEL	310.9–422.0	3	nosp	99.7	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.103.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
62GOL/BEL	310.9–422.0	3	1.00#	1.781	1.11	1.78	–4.02–1	–1
63GUD/CAM	313.1–483.1	4	1.00#	1.206	8.10–1	1.21	3.54–1	0

TABLE 12.103.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	1.751	1.13	1.75	3.00–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		1.54668+1	1.17371+1				V

TABLE 12.103.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.84	1.88	1.92	1.96	2.01	2.05	2.09
C_p (J K^{-1}mol^{-1})	431	441	451	460	470	480	490
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.13	2.17	2.21	2.26	2.30	2.34	2.38
C_p (J K^{-1}mol^{-1})	499	509	519	529	538	548	558
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.42	2.46	2.51	2.55			
C_p (J K^{-1}mol^{-1})	568	578	587	597			

Name: Bis(ethylcyclohexyl)methane (unspecified isomer)
Formula: $C_{17}H_{32}$

CAS-RN: 98028-64-9
Group No.: 12-104
Molar Mass: 236.44

TABLE 12.104.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	N	313.1–483.1	4	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 58.8 % of major component (not specified)

TABLE 12.104.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.719	4.97–1	0.72	1.81–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		2.38015+1	1.03230+1				V

TABLE 12.104.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.96	2.00	2.03	2.07	2.11	2.14	2.18
C_p (J K^{-1}mol^{-1})	464	473	481	490	498	507	515
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.22	2.25	2.29	2.33	2.36	2.40	2.43
C_p (J K^{-1}mol^{-1})	524	533	541	550	558	567	576
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.47	2.51	2.54	2.58			
C_p (J K^{-1}mol^{-1})	584	593	601	610			

Name: 1–Cyclohexyl–1–(1–methylethyl)cyclohexylethane (unspecified isomer)
Formula: $C_{17}H_{32}$

CAS-RN: 26637–18–3
Group No.: 12–105
Molar Mass: 236.44

TABLE 12.105.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	N	313.1–483.1	4	nosp	99.5	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 65.1 mol.% of major component (not specified)

TABLE 12.105.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.213	1.41–1	0.21	1.66–4	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		1.79794+1	1.22042+1				V

TABLE 12.105.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.96	2.01	2.05	2.09	2.13	2.18	2.22
C_p ($J K^{-1} mol^{-1}$)	464	474	484	494	505	515	525
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.26	2.31	2.35	2.39	2.43	2.48	2.52
C_p ($J K^{-1} mol^{-1}$)	535	545	555	566	576	586	596
Temp. (K)	450	460	470	480			
c_p ($J K^{-1} g^{-1}$)	2.56	2.61	2.65	2.69			
C_p ($J K^{-1} mol^{-1}$)	606	616	626	637			

Name: 3–Ethylhexadecahydropyrene
Formula: $C_{18}H_{30}$

CAS-RN: 94262–24–5
Group No.: 12–106
Molar Mass: 246.44

TABLE 12.106.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.9	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.106.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	1.024	6.10–1	1.02	5.09–3	1
Temp. range K		A_1	A_2				Level of uncertainty
310.9–422.0		3.03179+1	7.96830				IV

TABLE 12.106.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.856	1.883	1.910	1.937	1.964	1.991	2.018
C_p (J K^{-1}mol^{-1})	457.5	464.1	470.7	477.3	484.0	490.6	497.2
Temp. (K)	380	390	400	410	420		
c_p (J K^{-1}g^{-1})	2.044	2.071	2.098	2.125	2.152		
C_p (J K^{-1}mol^{-1})	503.8	510.5	517.1	523.7	530.3		

Name: 1-Cyclohexyloctahydro-1,3,3-trimethyl-1*H*-indene
Formula: $C_{18}H_{32}$

CAS-RN: 22236-61-9
Group No.: 12-107
Molar Mass: 248.45

TABLE 12.107.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.3	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	97.3	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.107.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.337	2.24–1	0.34	–4.54–2	–1
63GUD/CAM	313.1–483.1	4	1.00#	0.264	1.78–1	0.26	3.51–2	0

TABLE 12.107.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.352	2.36–1	0.35	6.03–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		9.46173	1.46815+1				IV

TABLE 12.107.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.840	1.889	1.938	1.987	2.036	2.085	2.135
C_p (J K^{-1}mol^{-1})	457.1	469.3	481.5	493.7	505.9	518.1	530.3
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.184	2.233	2.282	2.331	2.380	2.429	2.478
C_p (J K^{-1}mol^{-1})	542.5	554.7	566.9	579.2	591.4	603.6	615.8
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.528	2.577	2.626	2.675			
C_p (J K^{-1}mol^{-1})	628.0	640.2	652.4	664.6			

Name: 1,1':2',1''–Tercyclohexane
Formula: $C_{18}H_{32}$

CAS-RN: 2456–43–1
Group No.: 12–108
Molar Mass: 248.45

TABLE 12.108.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	97.8	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	95.6	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.108.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.261	1.55–1	0.26	1.51–1	3
63GUD/CAM	313.1–483.1	4	1.00#	0.877	5.20–1	0.88	–9.75–2	2

TABLE 12.108.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.810	4.80–1	0.81	9.07–3	5
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		5.86940	1.44709+1				V

TABLE 12.108.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.70	1.75	1.79	1.84	1.89	1.94	1.99
C_p (J K^{-1}mol^{-1})	422	434	446	458	470	482	494
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.04	2.09	2.13	2.18	2.23	2.28	2.33
C_p (J K^{-1}mol^{-1})	506	518	530	542	554	566	578
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.38	2.42	2.47	2.52			
C_p (J K^{-1}mol^{-1})	590	602	614	626			

Name: 1,1':3',1''–Tercyclohexane
Formula: $C_{18}H_{32}$

CAS-RN: 1706–50–9
Group No.: 12–109
Molar Mass: 248.45

TABLE 12.109.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	373.1–483.1	3	nosp	97.7	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.109.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.940	5.79–1	0.94	–1.01–1	–1
63GUD/CAM	373.1–483.1	3	1.00#	0.906	6.11–1	0.91	1.28–1	1

TABLE 12.109.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.306	8.41–1	1.31	1.34–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
310.9–483.1		9.06303+1	–2.69194+1	5.00584			V

TABLE 12.109.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.85	1.87	1.88	1.91	1.93	1.96	1.99
C_p (J K^{-1}mol^{-1})	460	464	468	474	480	487	495
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.03	2.07	2.11	2.16	2.20	2.26	2.31
C_p (J K^{-1}mol^{-1})	504	514	524	536	548	561	575
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.37	2.43	2.50	2.57			
C_p (J K^{-1}mol^{-1})	589	605	621	638			

Name: 1,1':4',1''–Tercyclohexane
Formula: $C_{18}H_{32}$

CAS-RN: 1795–19–3
Group No.: 12–110
Molar Mass: 248.45

TABLE 12.110.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	423.15	2.272	nosp	91.7	chrom	C_p	BDHT	63GUD/CAM

Name: 1,1–Bis(ethylcyclohexyl)ethane (unspecified isomer)
Formula: $C_{18}H_{34}$

CAS-RN: 98803–07–7
Group No.: 12–111
Molar Mass: 250.47

TABLE 12.111.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	N	313.1–483.1	4	nosp	97.9	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 78.8 % of major component (not specified)

TABLE 12.111.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.303	9.36–1	1.30	5.28–3	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		1.82936+1	1.26410+1				V

TABLE 12.111.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J $K^{-1}g^{-1}$)	1.91	1.95	1.99	2.03	2.08	2.12	2.16
C_p (J $K^{-1}mol^{-1}$)	478	488	499	509	520	530	541
Temp. (K)	380	390	400	410	420	430	440
c_p (J $K^{-1}g^{-1}$)	2.20	2.24	2.29	2.33	2.37	2.41	2.45
C_p (J $K^{-1}mol^{-1}$)	551	562	573	583	594	604	615
Temp. (K)	450	460	470	480			
c_p (J $K^{-1}g^{-1}$)	2.50	2.54	2.58	2.62			
C_p (J $K^{-1}mol^{-1}$)	625	636	646	657			

Name: 1,1,–Bis(dimethylcyclohexyl)ethane (unspecified isomer)
Formula: $C_{18}H_{34}$

CAS-RN: 98803–06–6
Group No.: 12–112
Molar Mass: 250.47

TABLE 12.112.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	N	313.1–483.1	4	nosp	99.0	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 57.3 % of major component (not specified)

TABLE 12.112.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.611	4.32–1	0.61	9.60–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		–2.90192+1	3.47508+1	–2.47710			V

TABLE 12.112.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.82	1.89	1.95	2.01	2.07	2.12	2.18
C_p (J K^{-1}mol^{-1})	456	472	488	503	518	532	546
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.23	2.28	2.34	2.38	2.43	2.48	2.52
C_p (J K^{-1}mol^{-1})	559	572	585	597	609	620	631
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.56	2.60	2.64	2.68			
C_p (J K^{-1}mol^{-1})	642	652	662	671			

Name: Dodecylcyclohexane
Formula: $C_{18}H_{36}$

CAS-RN: 1795–17–1
Group No.: 12–113
Molar Mass: 252.48

TABLE 12.113.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49PAR/MOO	290.0–300.0	2S	1.00	98.8	melpt	C_p	BSIO	25PAR

TABLE 12.113.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	1.91–6	0
Temp. range K		A_1	A_2				Level of uncertainty
290.0–300.0		3.25258+1	1.01643+1				IV

TABLE 12.113.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	2.042	2.069	2.075
C_p (J K^{-1}mol^{-1})	515.5	522.4	524.0

Name: Hexaethylcyclohexane (unspecified isomer)
Formula: $C_{18}H_{36}$

CAS-RN: 98803–61–3
Group No.: 12–114
Molar Mass: 252.48

TABLE 12.114.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	N	313.1–483.1	4	nosp	99.0	chrom	C_p	BDHT	63GUD/CAM

63GUD/CAM sample contained 47.7 % of 1,2,3,4,5,6–Hexaethylcyclohexane

TABLE 12.114.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	2.149	1.57	2.15	2.57–2	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		2.98133+1	1.11418+1				V

TABLE 12.114.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	2.12	2.16	2.19	2.23	2.27	2.30	2.34
C_p ($J K^{-1} mol^{-1}$)	535	544	554	563	572	581	591
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.38	2.41	2.45	2.49	2.52	2.56	2.60
C_p ($J K^{-1} mol^{-1}$)	600	609	618	628	637	646	655
Temp. (K)	450	460	470	480			
c_p ($J K^{-1} g^{-1}$)	2.63	2.67	2.71	2.74			
C_p ($J K^{-1} mol^{-1}$)	665	674	683	693			

Name: Bis(2,4,6–trimethylcyclohexyl)methane
Formula: $C_{19}H_{36}$

CAS-RN: 94380–80–0
Group No.: 12–115
Molar Mass: 264.49

TABLE 12.115.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63GUD/CAM	373.1–483.1	3	nosp	99.0	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.115.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	1.183	9.02–1	1.18	8.72–3	1
Temp. range K		A_1	A_2				Level of uncertainty
373.1–483.1		2.89109+1	1.12055+1				V

TABLE 12.115.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.21	2.25	2.28	2.32	2.35	2.39	2.42
C_p (J K^{-1}mol^{-1})	585	594	604	613	622	632	641
Temp. (K)	440	450	460	470	480		
c_p (J K^{-1}g^{-1})	2.46	2.49	2.53	2.56	2.60		
C_p (J K^{-1}mol^{-1})	650	660	669	678	688		

Name: 4–Heptyl–1,1'–bicyclohexyl
Formula: $C_{19}H_{36}$

CAS-RN: 96667–88–8
Group No.: 12–116
Molar Mass: 264.49

TABLE 12.116.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	100.0	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.116.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.551	3.75–1	0.55	1.33–3	0
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		1.80496+1	1.28913+1				IV

TABLE 12.116.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.824	1.864	1.905	1.945	1.986	2.026	2.067
C_p (J K^{-1}mol^{-1})	482.3	493.1	503.8	514.5	525.2	535.9	546.7
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.107	2.148	2.188	2.229	2.269	2.310	2.350
C_p (J K^{-1}mol^{-1})	557.4	568.1	578.8	589.5	600.2	611.0	621.7
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.391	2.432	2.472	2.513			
C_p (J K^{-1}mol^{-1})	632.4	643.1	653.8	664.6			

Name: 1,1'–Heptylidenebiscyclohexane
Formula: $C_{19}H_{36}$

CAS-RN: 2090–15–5
Group No.: 12–117
Molar Mass: 264.49

TABLE 12.117.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	95.7	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	313.1–483.1	4	nosp	95.7	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.117.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.884	6.71–1	0.88	–2.85–1	–1
63GUD/CAM	313.1–483.1	4	1.00#	0.435	3.40–1	0.43	2.26–1	0

TABLE 12.117.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.787	6.02–1	0.79	7.16–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		2.52775+1	1.24652+1				V

TABLE 12.117.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.01	2.05	2.09	2.13	2.17	2.21	2.24
C_p (J K^{-1}mol^{-1})	531	542	552	563	573	583	594
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.28	2.32	2.36	2.40	2.44	2.48	2.52
C_p (J K^{-1}mol^{-1})	604	614	625	635	645	656	666
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.56	2.60	2.64	2.68			
C_p (J K^{-1}mol^{-1})	677	687	697	708			

Name: Diethylhexadecahydropyrene
Formula: $C_{20}H_{34}$

CAS-RN: 26446–93–5
Group No.: 12–118
Molar Mass: 274.49

TABLE 12.118.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.118.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.783	5.50–1	0.78	3.16–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		1.12014+2	–3.49886+1	6.06955			V

TABLE 12.118.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.87	1.88	1.90	1.91	1.94	1.96	1.99
C_p (J K^{-1}mol^{-1})	514	517	521	526	531	538	546
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.02	2.06	2.10	2.14	2.18	2.24	2.29
C_p (J K^{-1}mol^{-1})	555	564	575	587	600	614	628
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.35	2.41	2.47	2.54			
C_p (J K^{-1}mol^{-1})	644	661	679	698			

Name: 9-(2-Ethylhexyl)dodecahydrofluorene
Formula: $C_{21}H_{38}$

CAS-RN: 95135-48-1
Group No.: 12-119
Molar Mass: 290.53

TABLE 12.119.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	not specified		C_p	BDHT	63GUD/CAM

TABLE 12.119.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	4	1.673	1.32	1.67	2.68–2	2
Temp. range K		A_1	A_2				Level of uncertainty
313.1–483.1		3.31552+1	1.26149+1				V

TABLE 12.119.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.07	2.10	2.14	2.18	2.21	2.25	2.28
C_p (J K^{-1}mol^{-1})	601	611	622	632	643	653	664
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.32	2.36	2.39	2.43	2.47	2.50	2.54
C_p (J K^{-1}mol^{-1})	674	685	695	706	716	727	737
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.57	2.61	2.65	2.68			
C_p (J K^{-1}mol^{-1})	748	758	769	779			

Name: 1,1',1''-(1-Propanyl-2-ylidene)triscyclohexane
Formula: $C_{21}H_{38}$

CAS-RN: 55682-89-8
Group No.: 12-120
Molar Mass: 290.53

TABLE 12.120.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	373.1–483.1	3	nosp	99.1	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.120.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.671	5.67-1	0.67	1.28-3	-1
Temp. range K		A_1	A_2				Level of uncertainty
373.1–483.1		2.52463+1	1.38599+1				IV

TABLE 12.120.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1}g^{-1}$)	2.190	2.230	2.269	2.309	2.349	2.388	2.428
C_p ($J K^{-1}mol^{-1}$)	636.3	647.8	659.3	670.9	682.4	693.9	705.4
Temp. (K)	440	450	460	470	480		
c_p ($J K^{-1}g^{-1}$)	2.468	2.507	2.547	2.587	2.626		
C_p ($J K^{-1}mol^{-1}$)	717.0	728.5	740.0	751.5	763.1		

Name: 4-Nonyl-1,1'-bicyclohexyl
Formula: $C_{21}H_{40}$

CAS-RN: 95135-87-8
Group No.: 12-121
Molar Mass: 292.55

TABLE 12.121.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	313.1–483.1	4	nosp	99.3	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.121.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	4	1.154	9.05-1	1.15	4.80-3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
313.1–483.1		6.22338+1	-4.34298	2.05202			V

TABLE 12.121.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.95	1.97	2.00	2.02	2.05	2.08	2.11
C_p ($J K^{-1} mol^{-1}$)	569	577	584	592	600	609	617
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.14	2.17	2.21	2.24	2.28	2.32	2.35
C_p ($J K^{-1} mol^{-1}$)	627	636	646	656	667	678	689
Temp. (K)	450	460	470	480			
c_p ($J K^{-1} g^{-1}$)	2.39	2.44	2.48	2.52			
C_p ($J K^{-1} mol^{-1}$)	700	712	725	737			

Name: 4'–Heptyl–1,1':3',1''–tercyclohexane
Formula: $C_{25}H_{46}$

CAS–RN: unknown
Group No.: 12–122
Molar Mass: 346.64

TABLE 12.122.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62GOL/BEL	310.9–422.0	3	nosp	99.0	chrom	C_p	BDHT	63GUD/CAM
63GUD/CAM	373.1–483.1	3	nosp	99.0	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.122.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62GOL/BEL	310.9–422.0	3	1.00#	0.531	4.96–1	0.53	3.64–1	1
63GUD/CAM	373.1–483.1	3	1.00#	1.545	1.50	1.54	–3.09–1	1

TABLE 12.122.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.415	1.37	1.41	2.78–2	2
Temp. range K		A_1	A_2				Level of uncertainty
310.9–483.1		3.27457+1	1.53670+1				V

TABLE 12.122.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.93	1.96	2.00	2.04	2.08	2.11	2.15
C_p (J K^{-1}mol^{-1})	668	681	694	707	719	732	745
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.19	2.22	2.26	2.30	2.33	2.37	2.41
C_p (J K^{-1}mol^{-1})	758	771	783	796	809	822	834
Temp. (K)	450	460	470	480			
c_p (J K^{-1}g^{-1})	2.44	2.48	2.52	2.55			
C_p (J K^{-1}mol^{-1})	847	860	873	886			

Name: 4'–Nonyl–1,1':3',1''–tercyclohexane
Formula: $C_{27}H_{50}$

CAS–RN: unknown
Group No.: 12–123
Molar Mass: 374.69

TABLE 12.123.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GUD/CAM	373.1–483.1	3	nosp	96.8	chrom	C_p	BDHT	63GUD/CAM

TABLE 12.123.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.737	7.87–1	0.74	5.42–3	I
Temp. range K		A_1	A_2				Level of uncertainty
373.1–483.1		3.64436+1	1.65801+1				V

able 12.123.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.17	2.21	2.24	2.28	2.32	2.35	2.39
C_p (J K^{-1}mol^{-1})	813	827	841	854	868	882	896
Temp. (K)	440	450	460	470	480		
c_p (J K^{-1}g^{-1})	2.43	2.46	2.50	2.54	2.57		
C_p (J K^{-1}mol^{-1})	910	923	937	951	965		

Name: (1–Decylundecyl)cyclohexane
Formula: $C_{27}H_{54}$

CAS-RN: 6703–99–7
Group No.: 12–124
Molar Mass: 378.73

TABLE 12.124.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
49PAR/MOO	270.0–300.0	4S	nosp	not specified	C_p	BSIO	25PAR

TABLE 12.124.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.000	1.53–5	0.00	–7.63–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
270.0–300.0		–1.10918+2	1.25783+2	–1.90581+1			IV

TABLE 12.124.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	1.971	1.986	2.017	2.054	2.079	2.084
C_p ($J\,K^{-1}mol^{-1}$)	746.3	752.2	763.8	778.0	787.3	789.1

13. Unsaturated Aliphatic Hydrocarbons

In this family the temperature dependent data are available for 36 alkenes (including 10 dienes) and 2 alkynes.

Systematic measurements were carried out for 21 C_5 to C_{16} substances at BMB with the reported error of 0.2 % (47TOD/OLI, 55SCO/FIN, 57MCC/FIN1, 70MES/TOD). Later new data were published by the former BMB (now called NIPER) (90MES/TOD) for two new alkenes and the earlier measurements were revised for additional two compounds having a claimed error of 0.1 %. The Bartlesville results have been considered as highly reliable and have been used alone for producing the recommended values with exception of 1-pentene where also the less accurate high pressure data from CIPT (49SCH/SAG) have been included for increasing the upper temperature limit of the recommended values. For the industrially important isoprene the extensive measurements at NBSW (37BEK/WOO) have been discarded as the data differed considerably from the Bartlesville values. The latter laboratory contributed this discrepancy to possible dissolved impurities (up to 1.7 %) in the NBSW sample; the contents was estimated from the shift in the triple point temperature of the sample (70MES/TOD).

Several low temperature isoperibol calorimeters were developed at UCB (37EGA/KEM, 39POW/GIA, 45GUT/PIT) which were used for supplying data for lowest alkenes C_2H_4 to C_4H_8 with the stated error of 0.2 %. Lower molar mass isomers of alkenes, dienes and 1-butyne were also measured at SUC (31HUF/PAR, 36TOD/PAR), NBSW (44SCO/FER, 45SCO/MAY) and PSC (46AST/FIN, 47AST/SZA, 50AST/MAS); the data from these sources are all in agreement to about 1 % and this is reasonable considering the time period of the measurements. The above mentioned data have been supplemented by less accurate high pressure data measured at CITP (49SCH/SAG, 50AUE/SAG, 52SCH/SAG) having an uncertainty which we have estimated to be about 1.5 %. For 2-butyne the low temperature measurements from CITP (41YOS/OSB) have been till recently the only available source. Later data obtained at the University of Complutense, Madrid, Spain (92BAO/CAC) have not been considered in the final selection as they seemed to be less reliable than the previous source.

Measurements for 3,3-dimethyl-1-butene (38KEM/SHO) and for two isomers of diisobutylene (denoted in the original paper as low and high boiling isomers, 36PAR/TOD2) were performed at SUC. The two isomers were not, however, sufficiently identified in the latter paper; according to the published melting and normal boiling temperatures, we guessed that the low boiling isomer was 2,4,4-trimethyl-1-pentene and 2,4,4-trimethyl-2-pentene corresponded to the high boiling one.

The only diene above C_4, 1,5-hexadiene, was measured in the last century at THA using a drop calorimeter (*81VON).

Name: Ethene
Formula: C_2H_4

CAS-RN: 74–85–1
Group No.: 13–001
Molar Mass: 28.05

TABLE 13.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
28EUC/HAU	110.0–170.0	7S	nosp	not specified	C_{sat}	BSIO	28EUC/HAU
37EGA/KEM	106.7–168.7	12	nosp	99.999 melpt	C_p	BSIO	37GIA/EGA

TABLE 13.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37EGA/KEM	106.7–168.7	12	0.30#	0.374	9.11–3	0.11	2.05–5	–2
				Rejected data				
28EUC/HAU	(9.55–1, 10.32, 8.70–1, 6)							

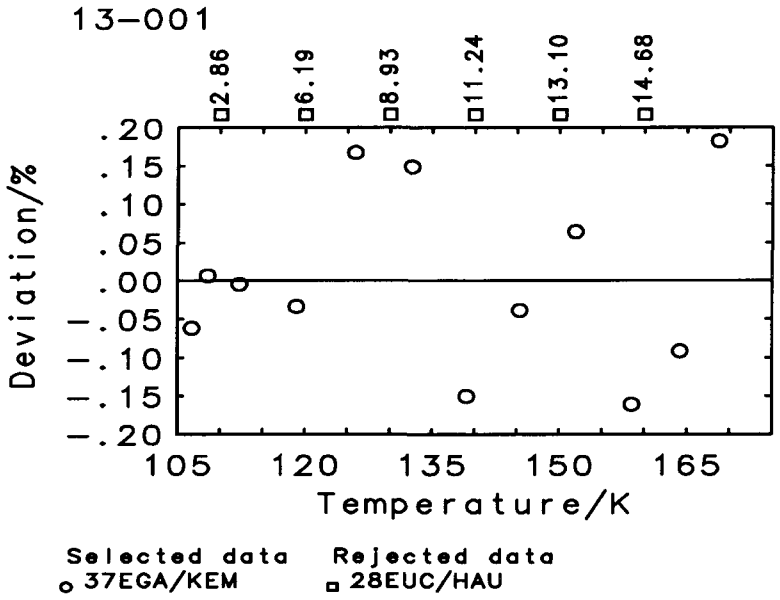
TABLE 13.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	12	0.431	1.05–2	0.13	2.05–5	–2
C_{sat}	19	12	0.425	1.04–2	0.13	1.95–5	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
106.7–168.7	1.00884+1	–2.48003	7.65137–1	III
106.7–168.7	9.95951	–2.27249	6.82698–1	III

TABLE 13.1.4. Recommended values of heat capacities

Temp. (K)	110	120	130	140	150	160	170
c_p (J K^{-1}g^{-1})	2.456	2.434	2.418	2.405	2.398	2.394	2.396
C_p (J K^{-1}mol^{-1})	68.90	68.30	67.83	67.48	67.26	67.17	67.21
c_{sat} (J K^{-1}g^{-1})	2.456	2.435	2.418	2.405	2.397	2.392	2.392
C_{sat} (J K^{-1}mol^{-1})	68.89	68.31	67.84	67.48	67.24	67.11	67.09



Name: 1–Propene
Formula: C_3H_6

CAS-RN: 115–07–1
Group No.: 13–002
Molar Mass: 42.08

TABLE 13.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31HUF/PAR	93.1–210.3	10	nosp	99.9	estim	C_p	BSIO	25PAR
39POW/GIA	93.9–223.4	18	0.20	99.978	melpt	C_p	BSIO	28GIA/WIE1
50AUE/SAG	299.8–344.3	9	3.00	not specified		C_p	BSAO	39SAG/EVA

TABLE 13.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
39POW/GIA	93.9–223.4	18	0.20	0.991	2.13–2	0.20	9.48–5	–1
50AUE/SAG	299.8–344.3	9	3.00	0.552	2.10–1	1.66	3.33–3	1
				Rejected data				
31HUF/PAR	(7.37–2, 0.70, –6.12–2, –6)							

TABLE 13.2.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	27	0.986	1.39–1	1.10	1.17–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
93.9–200.0		1.60047+1	–8.83788	4.41175	–6.55201–1		III
200.0–310.0		8.60837	2.25666	–1.13552	2.69344–1		IV
310.0–344.3		–3.19330+3	3.10087+3	–1.00069+3	1.07748+2		V

TABLE 13.2.3. Parameters of cubic spline polynomials

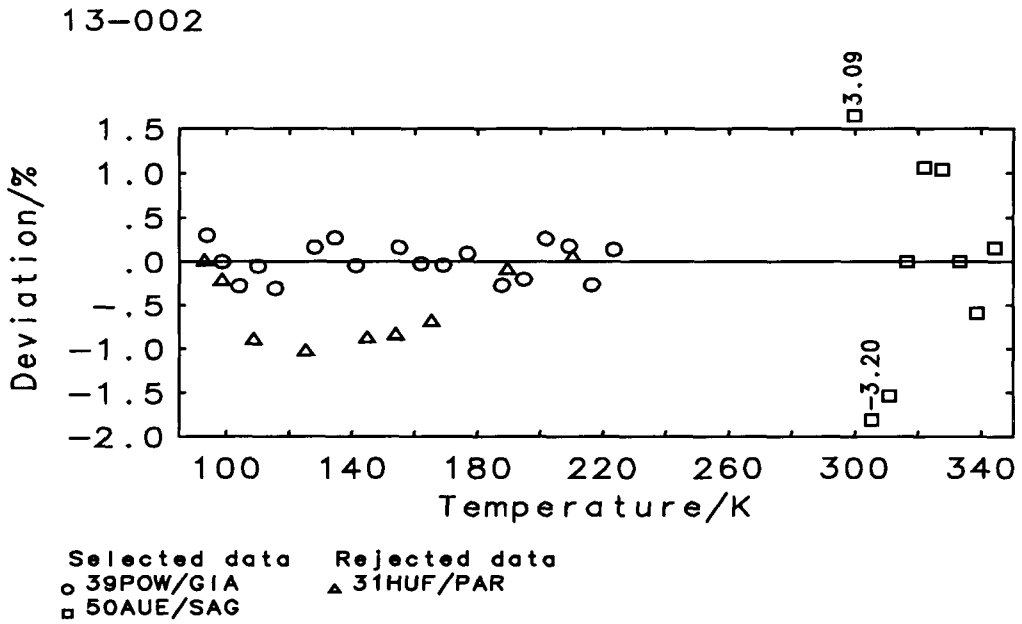
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	27	0.986	1.39–1	1.10	1.17–3	0
C_{sat}	37	27	0.988	1.37–1	1.11	2.69–3	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
93.9–200.0		1.60047+1	–8.83788	4.41175	–6.55201–1		III
200.0–310.0		8.60837	2.25666	–1.13552	2.69344–1		IV
310.0–344.3		–3.19330+3	3.10087+3	–1.00069+3	1.07748+2		V
93.9–200.0		1.60814+1	–9.01118	4.53842	–6.85168–1		III
200.0–310.0		1.07454+1	–1.00719	5.36424–1	–1.81681–2		IV
310.0–344.3		–2.41314+3	2.34469+3	–7.56139+2	8.13448+1		V

TABLE 13.2.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_p (J K^{-1}g^{-1})	2.202	2.158	2.124	2.098	2.081	2.071	2.067
C_p (J K^{-1}mol^{-1})	92.68	90.82	89.37	88.30	87.57	87.14	87.00
c_{sat} (J K^{-1}g^{-1})	2.203	2.158	2.124	2.098	2.081	2.071	2.067
C_{sat} (J K^{-1}mol^{-1})	92.69	90.82	89.37	88.29	87.56	87.14	87.00
Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	2.070	2.077	2.088	2.103	2.121	2.141	2.163
C_p (J K^{-1}mol^{-1})	87.09	87.40	87.88	88.51	89.25	90.08	91.00
c_{sat} (J K^{-1}g^{-1})	2.070	2.077	2.088	2.103	2.120	2.139	2.160
C_{sat} (J K^{-1}mol^{-1})	87.10	87.40	87.88	88.50	89.23	90.03	90.90
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.187	2.214	2.245	2.279	2.317	2.329	2.359
C_p (J K^{-1}mol^{-1})	92.03	93.18	94.47	95.90	97.49	98.02	99.25
c_{sat} (J K^{-1}g^{-1})	2.182	2.206	2.232	2.259	2.288	2.297	2.318
C_{sat} (J K^{-1}mol^{-1})	91.84	92.85	93.92	95.06	96.27	96.67	97.55
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.405	2.446	2.456	2.512	2.60	2.81	3.29
C_p (J K^{-1}mol^{-1})	101.2	102.9	103.4	105.7	109	118	138
c_{sat} (J K^{-1}g^{-1})	2.350	2.377	2.383	2.418	2.47	2.62	2.96
C_{sat} (J K^{-1}mol^{-1})	98.88	100.0	100.3	101.7	104	110	125
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	4.15						
C_p (J K^{-1}mol^{-1})	175						
c_{sat} (J K^{-1}g^{-1})	3.60						
C_{sat} (J K^{-1}mol^{-1})	151						

TABLE 13.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	20	1.663	2.81–1	2.04	–5.83–2	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
141.2–344.3	365.57	–2.88933–1	4.22652–1	9.55239	4.93799–2		V



Name: 1,2–Butadiene
Formula: C_4H_6

CAS-RN: 590–19–2
Group No.: 13–003
Molar Mass: 54.09

TABLE 13.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47AST/SZA	N	140.0–290.0	31S	0.20	99.89	melpt	C_p	BSAO	47AST/SZA

47AST/SZA errors below and above 200 K 0.1 % and 0.2 %, respectively

TABLE 13.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	31	0.377	1.02–2	0.08	1.21–5	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
140.0–290.0		1.61127+1	–3.51881	1.05399			III

TABLE 13.3.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p (J K^{-1}g^{-1})	2.037	2.030	2.026	2.025	2.028	2.034	2.043
C_p (J K^{-1}mol^{-1})	110.2	109.8	109.6	109.6	109.7	110.0	110.5
Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	2.055	2.071	2.090	2.112	2.137	2.166	2.197
C_p (J K^{-1}mol^{-1})	111.2	112.0	113.0	114.2	115.6	117.1	118.9
Temp. (K)	273.15	280	290	298.15			
c_p (J K^{-1}g^{-1})	2.208	2.232	2.271	2.304			
C_p (J K^{-1}mol^{-1})	119.4	120.8	122.8	124.6			

TABLE 13.3.5. Parameters of quasi-polynomial equation

Heat capacity type	*No. data points* total	used	s_w	*s/R*	s_r %	s_b/R	+/–
C_p	31	26	1.266	3.44–2	0.25	1.45–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
165.0–290.0	452.20	7.27575	4.08823	8.80550	3.23713		III

Name: 1,3–Butadiene
Formula: C_4H_6

CAS-RN: 106–99–0
Group No.: 13–004
Molar Mass: 54.09

TABLE 13.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
45SCO/MEY	165.0–300.0	29S	0.10	99.95	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 13.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	*s/R*	s_r %	s_b/R	+/–
C_p	29	29	0.697	9.54–3	0.07	1.77–5	1
C_{sat}	29	29	0.658	8.77–3	0.07	1.19–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
165.0–300.0		1.57459+1	–4.15515	1.30027			II
165.0–300.0		1.54941+1	–3.90430	1.23869			II

TABLE 13.4.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1}g^{-1}$)	1.912	1.918	1.928	1.942	1.960	1.983	2.009
C_p ($J K^{-1}mol^{-1}$)	103.4	103.8	104.3	105.1	106.0	107.2	108.6
c_{sat} ($J K^{-1}g^{-1}$)	1.912	1.918	1.929	1.943	1.961	1.983	2.009
C_{sat} ($J K^{-1}mol^{-1}$)	103.4	103.8	104.3	105.1	106.1	107.3	108.6
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	2.039	2.073	2.111	2.153	2.167	2.199	2.249
C_p ($J K^{-1}mol^{-1}$)	110.3	112.1	114.2	116.5	117.2	118.9	121.7
c_{sat} ($J K^{-1}g^{-1}$)	2.038	2.071	2.108	2.149	2.163	2.194	2.243
C_{sat} ($J K^{-1}mol^{-1}$)	110.2	112.0	114.0	116.3	117.0	118.7	121.3
Temp. (K)	298.15	300					
c_p ($J K^{-1}g^{-1}$)	2.293	2.303					
C_p ($J K^{-1}mol^{-1}$)	124.0	124.6					
c_{sat} ($J K^{-1}g^{-1}$)	2.285	2.295					
C_{sat} ($J K^{-1}mol^{-1}$)	123.6	124.1					

TABLE 13.4.5. *Parameters of quasi-polynomial equation*

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	29	2.842	3.73–2	0.28	1.71–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
165.0–300.0	425.17	1.87702	2.24415	9.44921	3.92485–1		III

Name: 1–Butyne
Formula: C_4H_6

CAS-RN: 107–00–6
Group No.: 13–005
Molar Mass: 54.09

TABLE 13.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
50AST/MAS	N	149.9–275.1	22	0.50	99.967	melpt	C_p	BSIO	36AST/MES

50AST/MAS errors below and above 200 K 0.3 % and 0.5 %, respectively

TABLE 13.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.593	4.44–2	0.30	2.28–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
149.9–275.1		1.65172+1	–3.73094	1.25624			III

TABLE 13.5.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	2.113	2.116	2.122	2.132	2.146	2.164	2.186
C_p (J K^{-1}mol^{-1})	114.3	114.4	114.8	115.3	116.1	117.1	118.3
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	2.212	2.241	2.275	2.312	2.353	2.398	2.413
C_p (J K^{-1}mol^{-1})	119.6	121.2	123.0	125.1	127.3	129.7	130.5
Temp. (K)	280						
c_p (J K^{-1}g^{-1})	2.447						
C_p (J K^{-1}mol^{-1})	132.4						

TABLE 13.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.717	5.42–2	0.36	3.23–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
149.9–275.1	463.70	1.30790+1	7.34862	6.05548	5.81948		III

Name: 2–Butyne
Formula: C_4H_6

CAS-RN: 503–17–3
Group No.: 13–006
Molar Mass: 54.09

TABLE 13.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
41YOS/OSB	N	249.5–284.3	10	0.20	99.75	melpt	C_p	BSAO	41YOS/GAR
92BAO/CAC		255.1–290.1	8	1.00	99.5	estim	C_p	BDHT	92BAO/CAC

41YOS/OSB C_p value at 255.06 K misprinted, 29.57 should read 28.57 cal/(K.mol)

TABLE 13.6.2. Correlated heat capacities

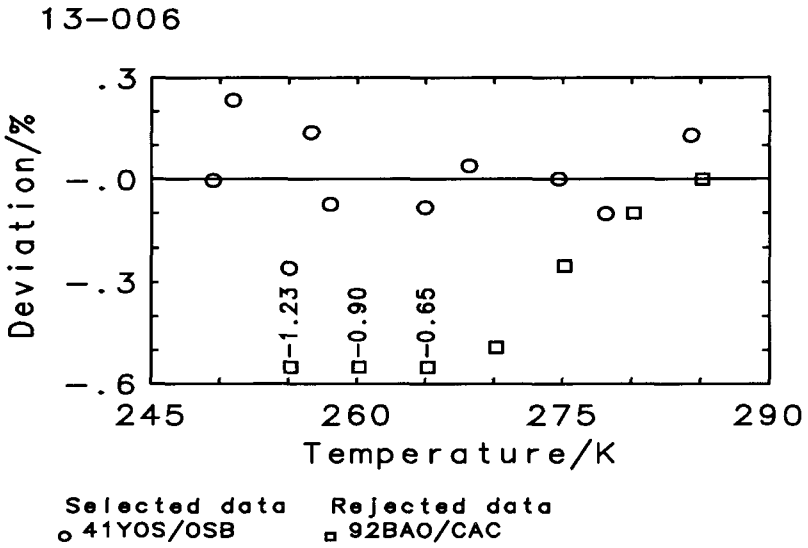
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41YOS/OSB	249.5–284.3	10	0.20	0.675	1.95–2	0.14	5.34–5	0
				Rejected data				
92BAO/CAC	(1.03–1, 0.72, –8.73–2, –6)							

TABLE 13.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	10	0.755	2.18–2	0.15	5.34–5	0
Temp. range K		A_1	A_2				Level of uncertainty
249.5–284.3		1.06547+1	1.47410				III

TABLE 13.6.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.204	2.227	2.250	2.257	2.272	2.295	2.313
C_p (J K^{-1}mol^{-1})	119.2	120.5	121.7	122.1	122.9	124.1	125.1



Name: 1–Butene
Formula: C_4H_8

CAS-RN: 106–98–9
Group No.: 13–007
Molar Mass: 56.11

TABLE 13.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36TOD/PAR		81.3–253.4	24	0.50	99.9	estim	C_p	BSIO	25PAR
46AST/FIN	N	89.8–258.5	18	0.30	99.54	melpt	C_p	BSIO	28GIA/WIE1
49SCH/SAG		310.9–366.5	11	1.50	not specified		C_p	BSAO	39SAG/EVA

46AST/FIN errors below and above 200 K 0.3 % and 0.5 %, respectively

TABLE 13.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
36TOD/PAR	81.3253.4	24	0.50	0.470	3.17–2	0.23	1.27–2	8
46AST/FIN	89.8–258.5	18	0.30	0.729	2.90–2	0.22	–5.12–3	0
49SCH/SAG	310.9–366.5	11	1.50	0.774	2.20–1	1.16	–2.52–2	–5

TABLE 13.7.3. Parameters of cubic spline polynomials

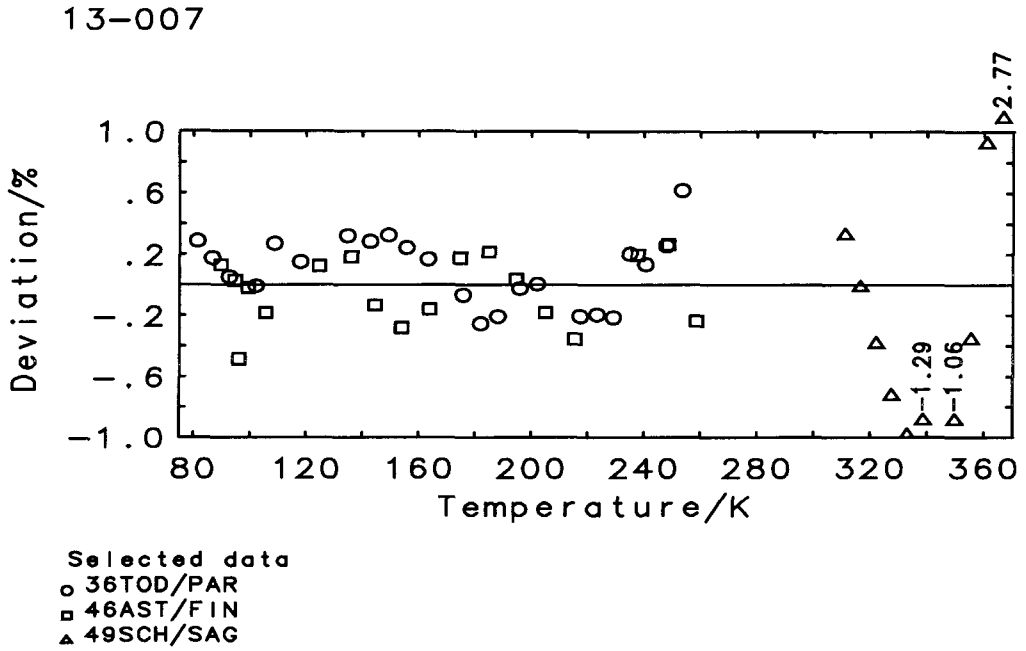
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	53	0.669	1.09–1	0.60	–1.23–3	3
C_{sat}	53	53	0.643	9.54–2	0.54	–9.01–5	5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
81.3–230.0		1.75376+1	–8.18394	4.17454	–5.76677–1		III
230.0–366.5		–3.18046	1.88397+1	–7.57486	1.12613		V
81.3–230.0		1.75357+1	–8.18299	4.17677	–5.77886–1		III
230.0–366.5		–7.33269–1	1.56460+1	–6.18368	9.23629–1		V

TABLE 13.7.4. Recommended values of heat capacities

Temp. (K)	90	100	110	120	130	140	150
c_p (J K^{-1}g^{-1})	1.946	1.919	1.900	1.887	1.880	1.879	1.883
C_p (J K^{-1}mol^{-1})	109.2	107.7	106.6	105.9	105.5	105.4	105.7
c_{sat} (J K^{-1}g^{-1})	1.946	1.919	1.900	1.887	1.880	1.879	1.883
C_{sat} (J K^{-1}mol^{-1})	109.2	107.7	106.6	105.9	105.5	105.4	105.7
Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.892	1.905	1.922	1.942	1.964	1.989	2.015
C_p (J K^{-1}mol^{-1})	106.2	106.9	107.8	108.9	110.2	111.6	113.1
c_{sat} (J K^{-1}g^{-1})	1.892	1.905	1.922	1.942	1.964	1.989	2.015
C_{sat} (J K^{-1}mol^{-1})	106.2	106.9	107.8	108.9	110.2	111.6	113.0
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.042	2.07	2.10	2.13	2.17	2.18	2.21
C_p (J K^{-1}mol^{-1})	114.6	116	118	120	122	122	124
c_{sat} (J K^{-1}g^{-1})	2.042	2.07	2.10	2.13	2.17	2.18	2.20
C_{sat} (J K^{-1}mol^{-1})	114.6	116	118	120	121	122	124
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.25	2.30	2.31	2.37	2.44	2.51	2.60
C_p (J K^{-1}mol^{-1})	127	129	129	133	137	141	146
c_{sat} (J K^{-1}g^{-1})	2.25	2.29	2.30	2.35	2.41	2.48	2.56
C_{sat} (J K^{-1}mol^{-1})	126	128	129	132	135	139	144
Temp. (K)	350	360	370				
c_p (J K^{-1}g^{-1})	2.70	2.82	2.94				
C_p (J K^{-1}mol^{-1})	152	158	165				
c_{sat} (J K^{-1}g^{-1})	2.65	2.75	2.86				
C_{sat} (J K^{-1}mol^{-1})	149	154	160				

TABLE 13.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	53	41	1.723	1.14–1	0.77	–1.76–2	–8
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
124.6–366.5	419.95	–1.35127	6.90682–1	1.08104+1	6.60913–1		V



Name: (*E*)–2–Butene
Formula: C_4H_8

CAS-RN: 624–64–6
Group No.: 13–008
Molar Mass: 56.11

TABLE 13.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36TOD/PAR	176.0–259.6	6	0.50	99.9	estim	C_p	BSIO	25PAR
45GUT/PIT	170.7–271.0	14	0.20	99.63	melpt	C_p	BSAO	45GUT/PIT

TABLE 13.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
45GUT/PIT	170.7–271.0	14	0.20	0.823	2.34–2	0.16	7.79–5	0
				Rejected data				
36TOD/PAR	(1.04–1, 0.72, 6.56–2, 2)							

TABLE 13.8.3. Parameters of regression polynomial

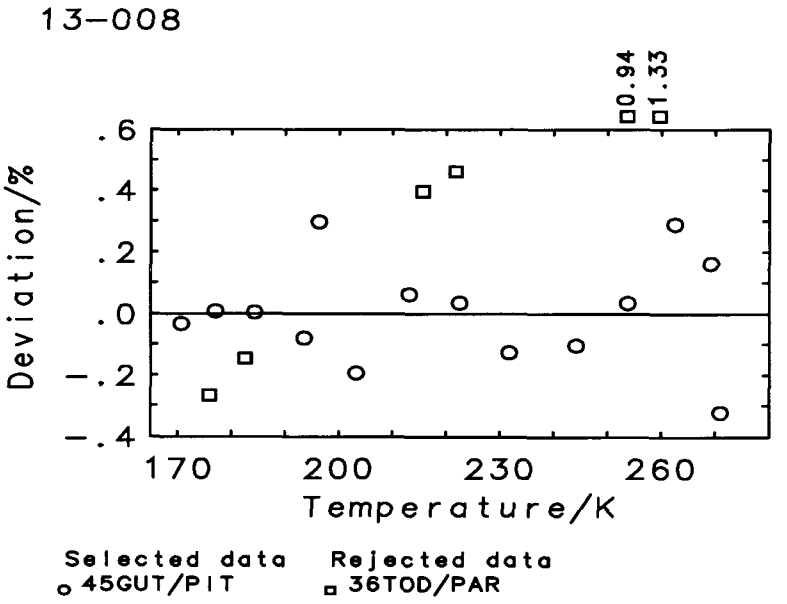
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	14	0.974	2.76–2	0.19	7.79–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
170.7–271.0		2.25852+1	−1.35561+1	6.16090	−8.24713−1		II

TABLE 13.8.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.970	1.976	1.988	2.003	2.023	2.045	2.069
C_p (J K^{-1}mol^{-1})	110.5	110.9	111.5	112.4	113.5	114.7	116.1
Temp. (K)	240	250	260	270			
c_p (J K^{-1}g^{-1})	2.095	2.121	2.148	2.173			
C_p (J K^{-1}mol^{-1})	117.5	119.0	120.5	121.9			

TABLE 13.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	14	1.445	4.07–2	0.29	1.83–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
170.7–271.0	428.63	−3.73205−1	1.20479	1.10428+1	2.89016−2		III



Name: (Z)–2–Butene
Formula: C_4H_8

CAS-RN: 590–18–1
Group No.: 13–009
Molar Mass: 56.11

TABLE 13.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36TOD/PAR	138.2–266.6	18	0.50	99.9	estim	C_p	BSIO	25PAR
44SCO/FER	134.3–300.0	36S	0.10	99.943	melpt	C_{sat}	BSAO	33SOU/BRI
52SCH/SAG	299.8–366.5	13S	1.50	99.8	estim	C_p	BSAO	39SAG/EVA

TABLE 13.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
44SCO/FER	134.3–300.0	36	0.10	0.866	1.26–2	0.09	–3.88–4	0
52SCH/SAG	299.8–366.5	13	1.50	1.046	2.71–1	1.57	2.66–1	13
				Rejected data				
36TOD/PAR	(7.51–2, 0.56, –6.96–2, –18)							

TABLE 13.9.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	67	49	0.968	1.47–1	0.86	7.03–2	13
C_{sat}	67	49	0.936	1.43–1	0.84	6.82–2	16

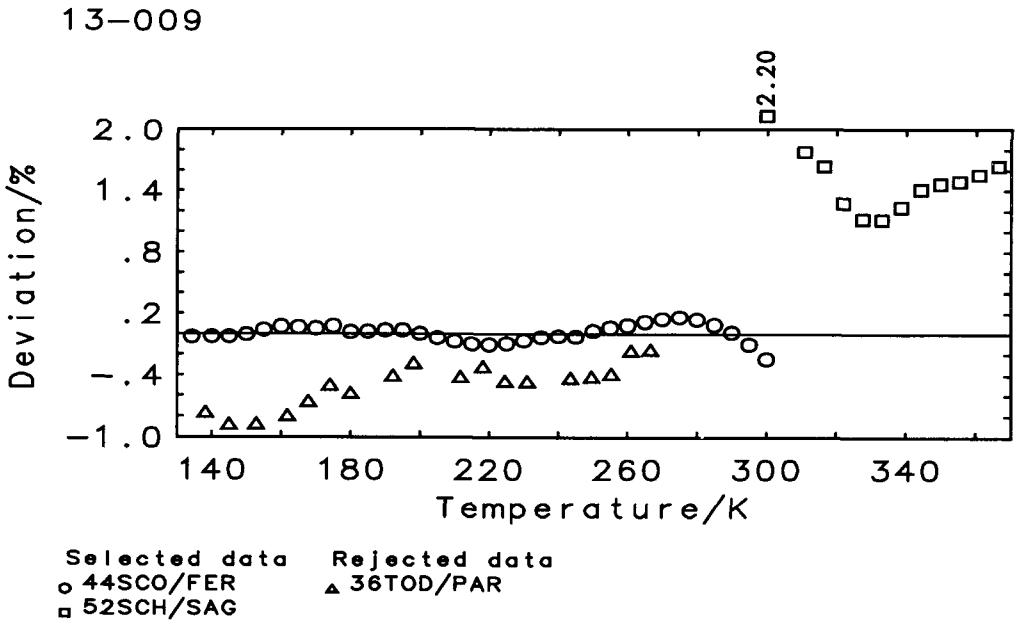
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
134.3–250.0	1.95676+1	–7.48436	2.60326	–2.00614–1	II
250.0–366.5	–3.45238	2.01396+1	–8.44634	1.27267	V
134.3–250.0	1.96826+1	–7.68436	2.71714	–2.21850–1	II
250.0–366.5	–1.39561	1.76095+1	–7.40041	1.12716	V

TABLE 13.9.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p (J K^{-1}g^{-1})	2.022	2.004	1.991	1.983	1.980	1.981	1.987
C_p (J K^{-1}mol^{-1})	113.4	112.4	111.7	111.3	111.1	111.2	111.5
c_{sat} (J K^{-1}g^{-1})	2.022	2.004	1.991	1.983	1.980	1.981	1.987
C_{sat} (J K^{-1}mol^{-1})	113.4	112.4	111.7	111.3	111.1	111.2	111.5
Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.997	2.010	2.028	2.049	2.074	2.10	2.13
C_p (J K^{-1}mol^{-1})	112.0	112.8	113.8	115.0	116.3	118	120
c_{sat} (J K^{-1}g^{-1})	1.997	2.010	2.028	2.049	2.073	2.10	2.13
C_{sat} (J K^{-1}mol^{-1})	112.0	112.8	113.8	114.9	116.3	118	120
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.15	2.17	2.22	2.26	2.27	2.33	2.40
C_p (J K^{-1}mol^{-1})	120	122	124	127	127	131	135
c_{sat} (J K^{-1}g^{-1})	2.14	2.17	2.21	2.25	2.26	2.32	2.39
C_{sat} (J K^{-1}mol^{-1})	120	122	124	126	127	130	134
Temp. (K)	330	340	350	360	370		
c_p (J K^{-1}g^{-1})	2.48	2.58	2.69	2.81	2.95		
C_p (J K^{-1}mol^{-1})	139	145	151	158	165		
c_{sat} (J K^{-1}g^{-1})	2.46	2.55	2.65	2.77	2.90		
C_{sat} (J K^{-1}mol^{-1})	138	143	149	155	162		

TABLE 13.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	67	43	2.984	8.23–2	0.51	2.03–2	9
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
160.0–366.5	435.58	–1.11740	5.11459–3	1.12695+1	1.69324+1	–5.24214+1	4.90685+1	V



Name: 2–Methyl–1–propene
Formula: C_4H_8

CAS-RN: 115–11–7
Group No.: 13–010
Molar Mass: 56.11

TABLE 13.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36TOD/PAR	139.2–253.1	15	0.50	99.9	estim	C_p	BSIO	25PAR

TABLE 13.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.158	1.09–2	0.08	1.29–5	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
139.2–253.1	1.49551+1	–3.91890	2.00970	–2.04006–1	III

TABLE 13.10.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p (J K^{-1}g^{-1})	1.904	1.913	1.926	1.941	1.959	1.981	2.004
C_p (J K^{-1}mol^{-1})	106.8	107.3	108.0	108.9	109.9	111.1	112.4

Temp. (K)	210	220	230	240	250
c_p (J K^{-1}g^{-1})	2.030	2.058	2.088	2.120	2.153
C_p (J K^{-1}mol^{-1})	113.9	115.5	117.2	118.9	120.8

TABLE 13.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.359	2.41–2	0.18	6.57–5	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
139.2–253.1	417.90	7.87193–1	2.14113	9.89321	7.23535–2	III

Name: 2–Methyl–1,3–butadiene
Formula: C_5H_8

CAS-RN: 78–79–5
Group No.: 13–011
Molar Mass: 68.12

TABLE 13.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37BEK/WOO	N	130.2–298.5	35	0.20	not specified		C_p	BSAO	33SOU/BRI
70MES/TOD		130.3–303.9	21	0.20	99.83	melpt	C_{sat}	BSAO	47HUF

37BEK/WOO impurity 1.7 mole % estimated by 70MES/TOD from triple point temperature

TABLE 13.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70MES/TOD	130.3–303.9	21	0.20#	0.112	3.59–3	0.02	4.54–8	–1
				Rejected data				
37BEK/WOO	(1.11–1, 0.66, 9.39–2, 32)							

TABLE 13.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	56	21	0.124	4.00–3	0.02	4.54–8	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
130.3–303.9	1.92297+1	–6.84607	2.94929	–2.59048–1			II

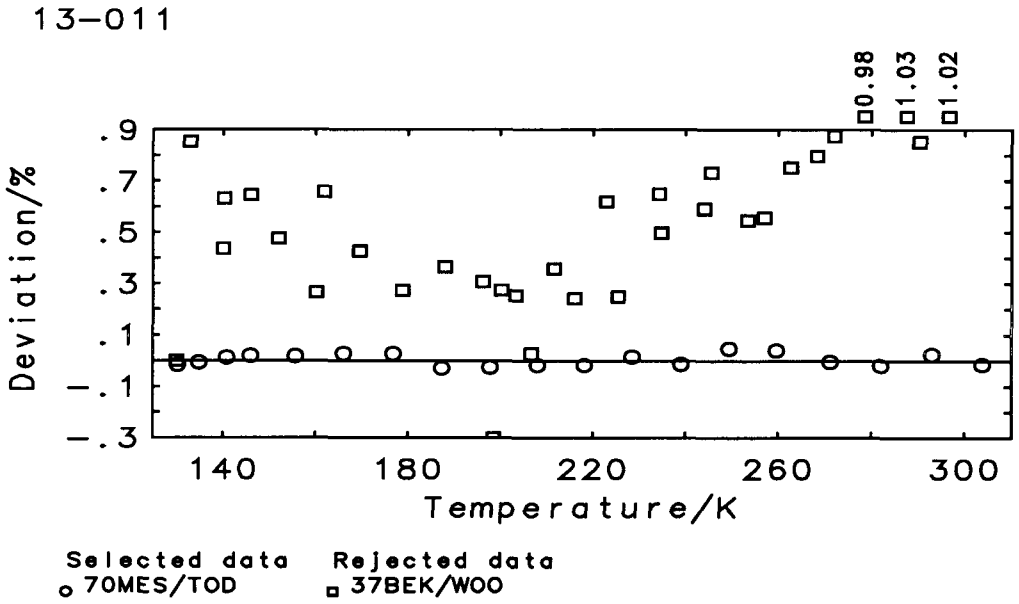
TABLE 13.11.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J K^{-1}g^{-1})	1.800	1.796	1.797	1.802	1.812	1.825	1.842
C_{sat} (J K^{-1}mol^{-1})	122.6	122.3	122.4	122.8	123.4	124.3	125.5
Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.863	1.887	1.914	1.945	1.978	2.014	2.052
C_{sat} (J K^{-1}mol^{-1})	126.9	128.5	130.4	132.5	134.7	137.2	139.8
Temp. (K)	270	273.15	280	290	298.15	300	
c_{sat} (J K^{-1}g^{-1})	2.093	2.106	2.136	2.180	2.218	2.226	
C_{sat} (J K^{-1}mol^{-1})	142.6	143.5	145.5	148.5	151.1	151.7	

TABLE 13.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	56	21	0.702	2.20–2	0.14	4.03–5	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
130.3–303.9	475.70	1.88933+2	1.58383+1	–2.59707	1.92529+2	–1.03593+1	1.94658+2	II



Name: 3–Methyl–1,2–butadiene
Formula: C_5H_8

CAS-RN: 598–25–4
Group No.: 13–012
Molar Mass: 68.12

TABLE 13.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70MES/TOD	161.9–314.6	20	0.20	99.98	melpt	C_{sat}	BSAO	47HUF

TABLE 13.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.091	3.04–3	0.02	7.15–7	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
161.9–314.6	1.75969+1	–3.35718	1.52343	–1.05608–1	II

TABLE 13.12.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.915	1.925	1.938	1.952	1.969	1.988	2.009
C_{sat} (J K^{-1}mol^{-1})	130.5	131.1	132.0	133.0	134.1	135.4	136.9
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	2.032	2.057	2.084	2.113	2.143	2.153	2.175
C_{sat} (J K^{-1}mol^{-1})	138.4	140.1	142.0	143.9	146.0	146.7	148.2
Temp. (K)	290	298.15	300	310			
c_{sat} (J K^{-1}g^{-1})	2.209	2.237	2.244	2.281			
C_{sat} (J K^{-1}mol^{-1})	150.5	152.4	152.9	155.3			

TABLE 13.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	20	20	0.990	3.35–2	0.20	1.05–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
161.9–314.6	489.20	–8.11580–1	2.05912	1.22293+1	7.99687–2		II

Name: 1,2-Pentadiene
Formula: C_5H_8

CAS-RN: 591-95-7
Group No.: 13-013
Molar Mass: 68.12

TABLE 13.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70MES/TOD	142.3–307.5	21	0.20	99.92	melpt	C_{sat}	BSAO	47HUF

TABLE 13.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	21	21	0.077	2.48–3	0.02	1.59–6	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
142.3–307.5		1.92139+1	–5.03246	2.06721	–1.67635–1		II

TABLE 13.13.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.924	1.923	1.925	1.930	1.938	1.949	1.962
C_{sat} (J K^{-1}mol^{-1})	131.0	131.0	131.1	131.4	132.0	132.7	133.7
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.979	1.997	2.018	2.042	2.067	2.094	2.123
C_{sat} (J K^{-1}mol^{-1})	134.8	136.0	137.5	139.1	140.8	142.7	144.6
Temp. (K)	273.15	280	290	298.15	300	310	
c_{sat} (J K^{-1}g^{-1})	2.133	2.154	2.187	2.215	2.221	2.256	
C_{sat} (J K^{-1}mol^{-1})	145.3	146.8	149.0	150.8	151.3	153.7	

TABLE 13.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.414	1.37–2	0.08	2.67–5	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
142.3–307.5	491.20	1.44883+2	1.21353+1	2.47926	1.47582+2	–7.78539	1.49292+2	II

Name: (*E*)–1,3–Pentadiene
Formula: C_5H_8

CAS-RN: 2004–70–8
Group No.: 13–014
Molar Mass: 68.12

TABLE 13.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70MES/TOD	189.2–316.4	17	0.20	99.9	melpt	C_{sat}	BSAO	47HUF

TABLE 13.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.347	1.11–2	0.07	1.17–5	–1
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
189.2–316.4	2.58705+1	–1.28646+1	4.84097	–4.74840–1	II

TABLE 13.14.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.910	1.917	1.929	1.946	1.967	1.991	2.020
C_{sat} (J K^{-1}mol^{-1})	130.1	130.6	131.4	132.6	134.0	135.7	137.6
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	2.051	2.085	2.096	2.121	2.160	2.193	2.200
C_{sat} (J K^{-1}mol^{-1})	139.7	142.0	142.8	144.5	147.1	149.4	149.9
Temp. (K)	310						
c_{sat} (J K^{-1}g^{-1})	2.242						
C_{sat} (J K^{-1}mol^{-1})	152.7						

TABLE 13.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.552	1.78–2	0.11	4.31–5	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
189.2–316.4	487.20	1.65500+2	1.28633+1	–3.45211–1	1.85567+2	–5.42808+1	2.12088+2	II

Name: (Z)–1,3–Pentadiene
Formula: C_5H_8

CAS-RN: 1574–41–0
Group No.: 13–015
Molar Mass: 68.12

TABLE 13.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70MES/TOD	138.2–316.1	22	0.20	99.91	melpt	C_{sat}	BSAO	47HUF

TABLE 13.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.079	2.50–3	0.02	–1.04–6	3
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
138.2–316.1	2.20720+1	–8.31741	2.99909	–2.37835–1	II

TABLE 13.15.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.911	1.897	1.888	1.884	1.883	1.888	1.896
C_{sat} (J K^{-1}mol^{-1})	130.1	129.2	128.6	128.3	128.3	128.6	129.1
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.908	1.923	1.942	1.965	1.990	2.019	2.050
C_{sat} (J K^{-1}mol^{-1})	129.9	131.0	132.3	133.8	135.6	137.5	139.7
Temp. (K)	273.15	280	290	298.15	300	310	
c_{sat} (J K^{-1}g^{-1})	2.061	2.084	2.121	2.152	2.159	2.200	
C_{sat} (J K^{-1}mol^{-1})	140.4	142.0	144.5	146.6	147.1	149.9	

TABLE 13.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	16	0.411	1.34–2	0.08	1.09–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
173.6–316.1	490.20	1.63995+2	1.27573+1	–5.33111–1	1.85335+2	–5.71994+1	2.12098+2	II

Name: 1,4–Pentadiene
Formula: C_5H_8

CAS-RN: 591–93–5
Group No.: 13–016
Molar Mass: 68.12

TABLE 13.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36PAR/TOD2	125.4–292.5	23	0.50	99.9	melpt	C_p	BSIO	25PAR
70MES/TOD	128.0–300.9	22	0.20	99.98	melpt	C_{sat}	BSAO	47HUF

TABLE 13.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70MES/TOD	128.0–300.9	22	0.20#	0.106	3.30–3	0.02	3.08–6	3
				Rejected data				
36PAR/TOD2	(6.45–2, 0.38, 1.98–2, 3)							

TABLE 13.16.3. Parameters of regression polynomial

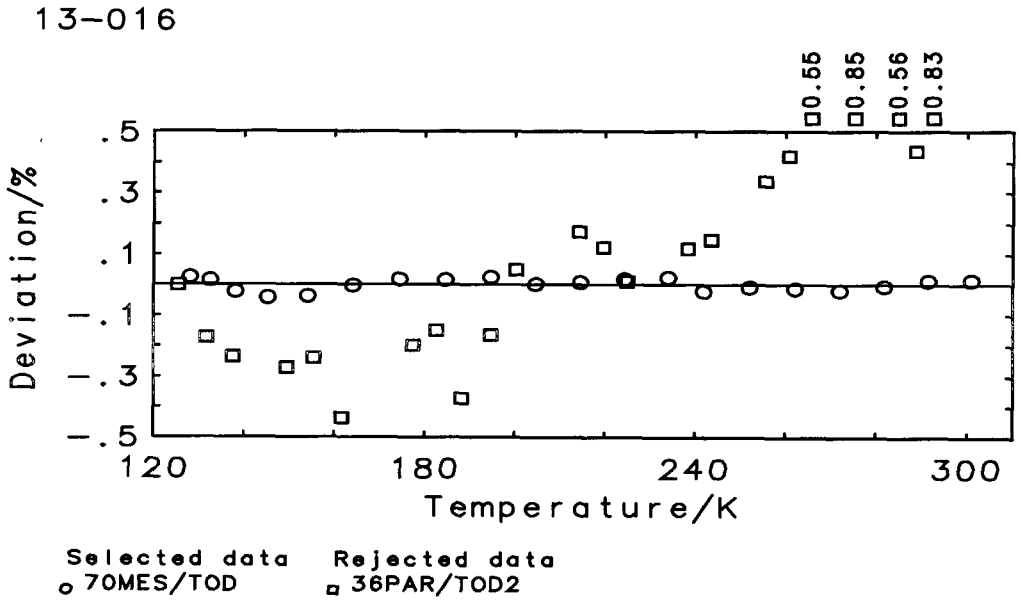
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	45	22	0.117	3.65–3	0.02	3.08–6	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
128.0–300.9		1.96736+1	–6.11737	2.40621	–1.95032–1		II

TABLE 13.16.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J K^{-1}g^{-1})	1.875	1.866	1.862	1.861	1.864	1.870	1.880
C_{sat} (J K^{-1}mol^{-1})	127.7	127.1	126.8	126.8	127.0	127.4	128.0
Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.892	1.908	1.927	1.948	1.972	1.998	2.027
C_{sat} (J K^{-1}mol^{-1})	128.9	130.0	131.2	132.7	134.3	136.1	138.1
Temp. (K)	270	273.15	280	290	298.15	300	
c_{sat} (J K^{-1}g^{-1})	2.058	2.068	2.091	2.125	2.155	2.162	
C_{sat} (J K^{-1}mol^{-1})	140.2	140.9	142.4	144.8	146.8	147.3	

TABLE 13.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	45	16	0.325	1.04–2	0.07	1.07–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
154.1–300.9	462.20	8.60776+1	6.17988	7.68986	9.58082+1	–2.82775+1	1.18011+2	II



Name: 2,3–Pentadiene
Formula: C_5H_8

CAS-RN: 591–96–8
Group No.: 13–017
Molar Mass: 68.12

TABLE 13.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70MES/TOD	150.7–315.1	21	0.20	99.88	melpt	C_{sat}	BSAO	47HUF

TABLE 13.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.078	2.60–3	0.02	8.17–7	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
150.7–315.1		1.93375+1	–4.04968	1.49720	–8.48617–2		II

TABLE 13.17.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J K^{-1}g^{-1})	1.995	1.995	1.997	2.002	2.010	2.020	2.032
C_{sat} (J K^{-1}mol^{-1})	135.9	135.9	136.1	136.4	136.9	137.6	138.4
Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	2.047	2.064	2.083	2.105	2.128	2.154	2.163
C_{sat} (J K^{-1}mol^{-1})	139.4	140.6	141.9	143.4	145.0	146.7	147.3
Temp. (K)	280	290	298.15	300	310	320	
c_{sat} (J K^{-1}g^{-1})	2.182	2.211	2.237	2.242	2.276	2.310	
C_{sat} (J K^{-1}mol^{-1})	148.6	150.6	152.4	152.8	155.0	157.4	

TABLE 13.17.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.315	1.06–2	0.06	1.30–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
150.7–315.1	497.20	9.34029+1	6.99568	8.27198	9.97942+1	–1.89302+1	1.16200+2	II

Name: 2–Methyl–1–butene
Formula: C_5H_{10}

CAS–RN: 563–46–2
Group No.: 13–018
Molar Mass: 70.13

TABLE 13.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47TOD/OLI	140.1–292.9	23	0.20	99.95	melpt	C_{sat}	BSAO	47HUF

TABLE 13.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.126	4.20–3	0.03	2.65–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
140.1–292.9		1.94579+1	–5.09285	2.08121	–1.45714–1		II

TABLE 13.18.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.898	1.898	1.902	1.909	1.919	1.932	1.948
C_{sat} (J K^{-1}mol^{-1})	133.1	133.1	133.4	133.9	134.6	135.5	136.6
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.967	1.989	2.013	2.040	2.069	2.101	2.135
C_{sat} (J K^{-1}mol^{-1})	138.0	139.5	141.2	143.1	145.1	147.4	149.8
Temp. (K)	273.15	280	290	298.15			
c_{sat} (J K^{-1}g^{-1})	2.146	2.171	2.210	2.242			
C_{sat} (J K^{-1}mol^{-1})	150.5	152.3	155.0	157.2			

TABLE 13.18.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.352	1.16–2	0.07	1.27–5	–4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
140.1–292.9	470.20	1.37454+2	1.10921+1	3.64526	1.42489+2	–1.46131+1	1.51531+2	II

Name: 2–Methyl–2–butene
Formula: C_5H_{10}

CAS–RN: 513–35–9
Group No.: 13–019
Molar Mass: 70.13

TABLE 13.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
30PAR/HUF1	143.9–293.9	15	1.00	not specified	C_p	BSIO	25PAR
47TOD/OLI	140.9–301.0	24	0.20	99.95 melpt	C_{sat}	BSAO	47HUF

TABLE 13.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47TOD/OLI	140.9–301.0	24	0.20#	0.226	7.48–3	0.05	7.11–6	–1
				Rejected data				
30PAR/HUF1	(8.99–2, 0.52, –5.88–2, –10)							

TABLE 13.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	39	24	0.248	8.20–3	0.05	7.11–6	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
140.9–301.0	1.90849+1	–4.42379	1.65433	–8.39777–2			II

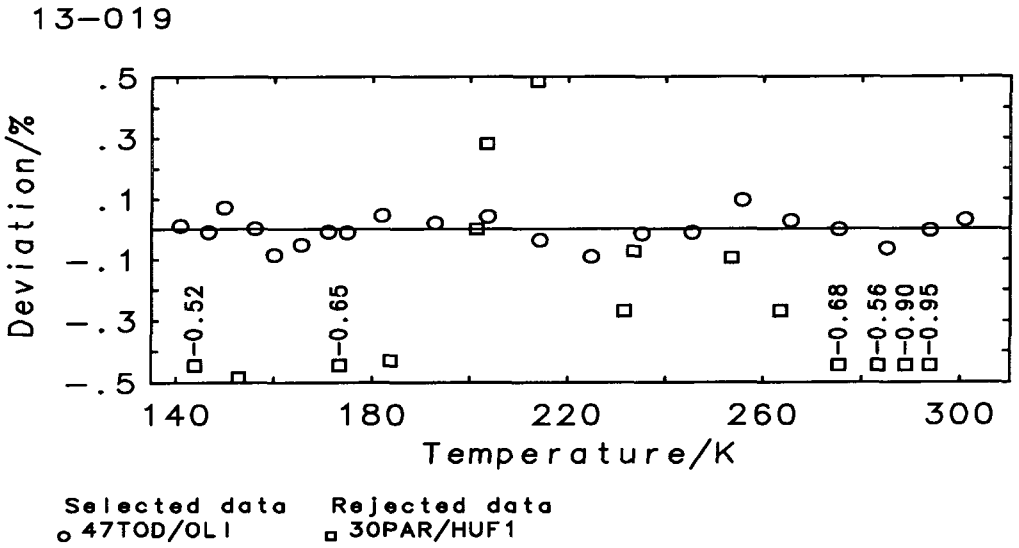
TABLE 13.19.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} ($J\,K^{-1}g^{-1}$)	1.885	1.884	1.885	1.889	1.896	1.906	1.918
C_{sat} ($J\,K^{-1}mol^{-1}$)	132.2	132.1	132.2	132.5	133.0	133.7	134.6
Temp. (K)	210	220	230	240	250	260	270
c_{sat} ($J\,K^{-1}g^{-1}$)	1.934	1.952	1.973	1.996	2.022	2.050	2.080
C_{sat} ($J\,K^{-1}mol^{-1}$)	135.6	136.9	138.4	140.0	141.8	143.8	145.9
Temp. (K)	273.15	280	290	298.15	300		
c_{sat} ($J\,K^{-1}g^{-1}$)	2.090	2.113	2.148	2.178	2.185		
C_{sat} ($J\,K^{-1}mol^{-1}$)	146.6	148.2	150.7	152.8	153.3		

TABLE 13.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	39	24	0.460	1.52–2	0.09	3.26–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
140.9–301.0	481.20	1.32943+2	1.05061+1	3.80543	1.41581+2	–2.45434+1	1.56121+2	II



Name: 3–Methyl–1–butene
Formula: C_5H_{10}

CAS–RN: 563–45–1
Group No.: 13–020
Molar Mass: 70.13

TABLE 13.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
47TOD/OLI	110.6–298.4	24	0.20	99.995	melpt	C_{sat}	BSAO	47HUF

TABLE 13.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.426	1.37–2	0.09	2.06–5	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
110.6–298.4	1.55001+1	–2.12757	1.26394	–6.20012–2	II

TABLE 13.20.4. Recommended values of heat capacities

Temp. (K)	110	120	130	140	150	160	170
c_{sat} (J K^{-1}g^{-1})	1.732	1.738	1.747	1.758	1.772	1.787	1.806
C_{sat} (J K^{-1}mol^{-1})	121.4	121.9	122.5	123.3	124.2	125.4	126.6
Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.826	1.849	1.874	1.901	1.930	1.961	1.994
C_{sat} (J K^{-1}mol^{-1})	128.1	129.7	131.4	133.3	135.3	137.5	139.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	2.029	2.066	2.104	2.117	2.145	2.187	2.223
C_{sat} (J K^{-1}mol^{-1})	142.3	144.9	147.6	148.5	150.4	153.4	155.9
Temp. (K)	300						
c_{sat} (J K^{-1}g^{-1})	2.231						
C_{sat} (J K^{-1}mol^{-1})	156.5						

TABLE 13.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.620	1.98–2	0.12	4.08–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
110.6–298.4	453.20	2.22495+1	1.12826	1.32620+1	2.12359+1	7.05572	3.16854+1	II

Name: 1-Pentene
Formula: C_5H_{10}

CAS-RN: 109-67-1
Group No.: 13-021
Molar Mass: 70.13

TABLE 13.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
47TOD/OLI	125.7–295.3	24	0.20	not specified		C_{sat}	BSAO	47HUF
49SCH/SAG	310.9–366.5	11	1.50	not specified		C_p	BSAO	39SAG/EVA
90MES/TOD	111.0–308.4	25	0.10	99.913	melpt	C_{sat}	BSAO	47HUF

TABLE 13.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47TOD/OLI	125.7–295.3	24	0.20	0.461	1.54–2	0.09	1.25–2	20
49SCH/SAG	310.9–366.5	11	1.50	0.572	1.70–1	0.86	–1.06–1	–7
90MES/TOD	111.0–308.4	25	0.10	0.535	9.51–3	0.05	–2.76–3	–13

TABLE 13.21.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	60	60	0.537	7.71–2	0.39	–1.57–2	0
C_{sat}	60	60	0.533	7.89–2	0.40	–1.62–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
111.0–300.0	1.81128+1	–4.16574	1.78245	–1.08500–1	I
300.0–366.5	1.17329+2	–1.03382+2	3.48544+1	–3.78316	V
111.0–300.0	1.82039+1	–4.32891	1.87602	–1.25713–1	I
300.0–366.5	1.26012+2	–1.12137+2	3.78119+1	–4.11859	V

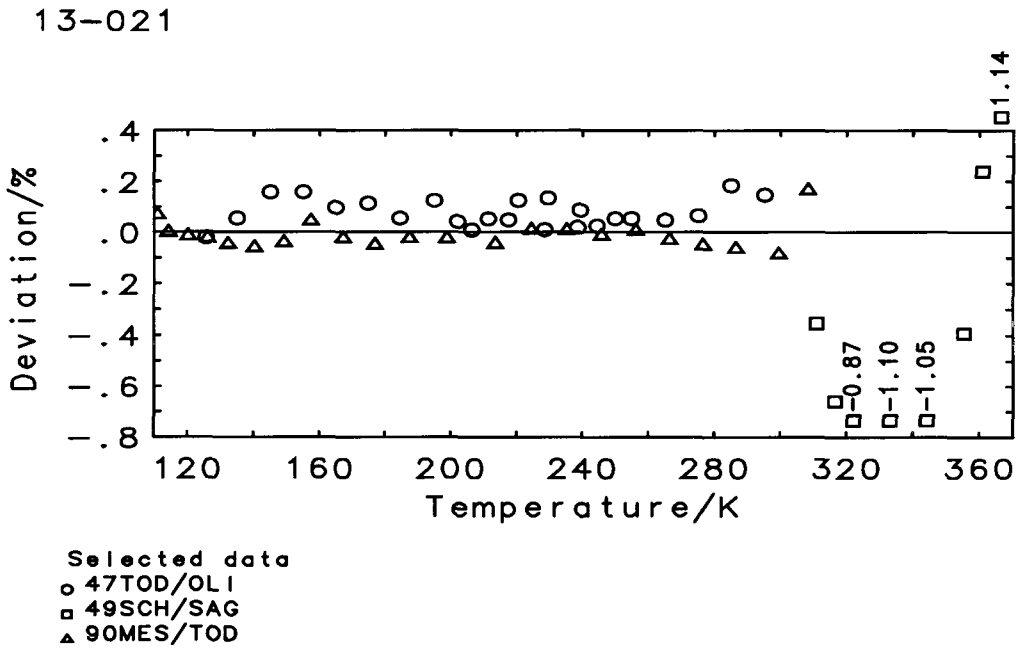
TABLE 13.21.4. Recommended values of heat capacities

Temp. (K)	110	120	130	140	150	160	170
c_p ($J K^{-1}g^{-1}$)	1.8426	1.8367	1.8341	1.8348	1.8386	1.8454	1.8552
C_p ($J K^{-1}mol^{-1}$)	129.23	128.82	128.64	128.68	128.95	129.43	130.12
c_{sat} ($J K^{-1}g^{-1}$)	1.8429	1.8368	1.8341	1.8346	1.8384	1.8453	1.8552
C_{sat} ($J K^{-1}mol^{-1}$)	129.25	128.82	128.63	128.67	128.94	129.42	130.11
Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1}g^{-1}$)	1.8680	1.8836	1.9019	1.9230	1.9466	1.9728	2.0014
C_p ($J K^{-1}mol^{-1}$)	131.01	132.10	133.39	134.87	136.52	138.36	140.37
c_{sat} ($J K^{-1}g^{-1}$)	1.8680	1.8837	1.9021	1.9232	1.9468	1.9729	2.0014
C_{sat} ($J K^{-1}mol^{-1}$)	131.01	132.11	133.40	134.88	136.54	138.37	140.37
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	2.0324	2.0657	2.1012	2.1128	2.1388	2.1785	2.2124
C_p ($J K^{-1}mol^{-1}$)	142.54	144.87	147.36	148.18	150.01	152.79	155.16
c_{sat} ($J K^{-1}g^{-1}$)	2.0323	2.0653	2.1004	2.1119	2.1376	2.1768	2.2100
C_{sat} ($J K^{-1}mol^{-1}$)	142.53	144.85	147.31	148.12	149.92	152.67	155.00
Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1}g^{-1}$)	2.2202	2.26	2.31	2.34	2.38	2.40	2.41
C_p ($J K^{-1}mol^{-1}$)	155.72	159	162	164	167	168	169
c_{sat} ($J K^{-1}g^{-1}$)	2.2177	2.26	2.30	2.34	2.37	2.39	2.40
C_{sat} ($J K^{-1}mol^{-1}$)	155.54	159	161	164	166	167	168

TABLE 13.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	60	60	2.082	4.70–2	0.27	–5.95–3	–18

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
111.0–366.5	464.78	5.22732+1	3.36498	1.17701+1	5.36613+1	–5.04617	7.09940+1	V



Name: 2–Pentene
Formula: C_5H_{10}

CAS–RN: 109–68–2
Group No.: 13–022
Molar Mass: 70.13

TABLE 13.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON N	296.8–306.0	4S	nosp	not specified		C_{avg}	DSIO	*81VON
30PAR/HUF1	136.1–289.1	8	1.00	not specified		C_p	BSIO	25PAR

*81VON substance not clearly identified, name "Amylen" used; probably 2–Pentene (according to n.b.t.)

TABLE 13.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	296.8–306.0	4	2.00#	0.593	2.26–1	1.19	1.93–1	4
30PAR/HUF1	136.1–289.1	8	1.00	0.385	6.75–2	0.38	–2.28–2	–4

TABLE 13.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.536	1.63–1	0.87	4.91–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
136.1–306.0		1.65680+1	–2.15818	9.55251–1			V

TABLE 13.22.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p ($J K^{-1} g^{-1}$)	1.83	1.84	1.84	1.86	1.87	1.89	1.91
C_p ($J K^{-1} mol^{-1}$)	128	129	129	130	131	132	134
Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1} g^{-1}$)	1.93	1.95	1.97	2.00	2.03	2.06	2.10
C_p ($J K^{-1} mol^{-1}$)	135	137	138	140	143	145	147
Temp. (K)	273.15	280	290	298.15	300	310	
c_p ($J K^{-1} g^{-1}$)	2.11	2.14	2.17	2.21	2.22	2.26	
C_p ($J K^{-1} mol^{-1}$)	148	150	153	155	155	158	

TABLE 13.22.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.489	1.09–1	0.61	–8.52–3	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
136.1–306.0	475.00	4.77990	4.68347	1.01201+1	1.21958		V

Name: (*E*)–2–Pentene
Formula: C_5H_{10}

CAS–RN: 646–04–8
Group No.: 13–023
Molar Mass: 70.13

TABLE 13.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
47TOD/OLI	135.0–301.7	27	0.20	99.995	melpt	C_{sat}	BSAO	47HUF

TABLE 13.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	27	0.270	9.20–3	0.05	7.31–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
135.0–301.7		1.59522+1	–1.61398	8.70985–1			II

TABLE 13.23.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.826	1.836	1.849	1.864	1.881	1.900	1.922
C_{sat} (J K^{-1}mol^{-1})	128.0	128.8	129.7	130.8	131.9	133.3	134.8
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.945	1.970	1.997	2.027	2.058	2.092	2.127
C_{sat} (J K^{-1}mol^{-1})	136.4	138.2	140.1	142.1	144.3	146.7	149.2
Temp. (K)	273.15	280	290	298.15	300		
c_{sat} (J K^{-1}g^{-1})	2.139	2.165	2.205	2.239	2.246		
C_{sat} (J K^{-1}mol^{-1})	150.0	151.8	154.6	157.0	157.6		

TABLE 13.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	27	27	1.131	3.86–2	0.23	1.39–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
135.0–301.7	474.20	–8.11492–2	2.76166	1.14140+1	5.96126–4		III

Name: (Z)–2–Pentene
Formula: C_5H_{10}

CAS–RN: 627–20–3
Group No.: 13–024
Molar Mass: 70.13

TABLE 13.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
47TOD/OLI	128.7–295.3	37	0.20	99.995	melpt	C_{sat}	BSAO	47HUF

TABLE 13.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	37	37	0.396	1.36–2	0.08	1.82–5	6
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
128.7–295.3		2.13097+1	–7.11514	2.58379	–1.81446–1		II

TABLE 13.24.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J K^{-1}g^{-1})	1.900	1.887	1.878	1.873	1.872	1.875	1.882
C_{sat} (J K^{-1}mol^{-1})	133.3	132.3	131.7	131.3	131.3	131.5	132.0
Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.892	1.907	1.924	1.945	1.969	1.996	2.026
C_{sat} (J K^{-1}mol^{-1})	132.7	133.7	134.9	136.4	138.1	140.0	142.1
Temp. (K)	270	273.15	280	290	298.15	300	
c_{sat} (J K^{-1}g^{-1})	2.058	2.069	2.094	2.132	2.164	2.172	
C_{sat} (J K^{-1}mol^{-1})	144.4	145.1	146.8	149.5	151.8	152.3	

TABLE 13.24.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	37	29	0.466	1.62–2	0.09	1.66–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
163.7–295.3	475.20	2.19302+2	1.83175+1	–6.45813	2.42391+2	–5.98522+1	2.57149+2	II

Name: 1,5-Hexadiene
Formula: C_6H_{10}

CAS-RN: 592-42-7
Group No.: 13-025
Molar Mass: 82.15

TABLE 13.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	297.0–309.7	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 13.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.003	1.38–3	0.01	–4.77–7	0
Temp. range K		A_1	A_2				Level of uncertainty
297.0–309.7		5.51252	5.21277				V

TABLE 13.25.4. Recommended values of heat capacities

Temp. (K)	300	310
c (J K^{-1}g^{-1})	2.14	2.19
C (J K^{-1}mol^{-1})	176	180

Name: 2,3–Dimethyl–2–butene
Formula: C_6H_{12}

CAS–RN: 563–79–1
Group No.: 13–026
Molar Mass: 84.16

TABLE 13.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
36PAR/TOD2	202.4–295.5	12	0.50	not specified	C_p	BSIO	25PAR
55SCO/FIN	204.3–318.1	18	0.20	99.95 melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 13.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
55SCO/FIN	204.3–318.1	18	0.20	0.071	2.74–3	0.01	–5.30–7	1
				Rejected data				
36PAR/TOD2	(1.35–1, 0.66, 1.22–1, 11)							

TABLE 13.26.3. Parameters of regression polynomial

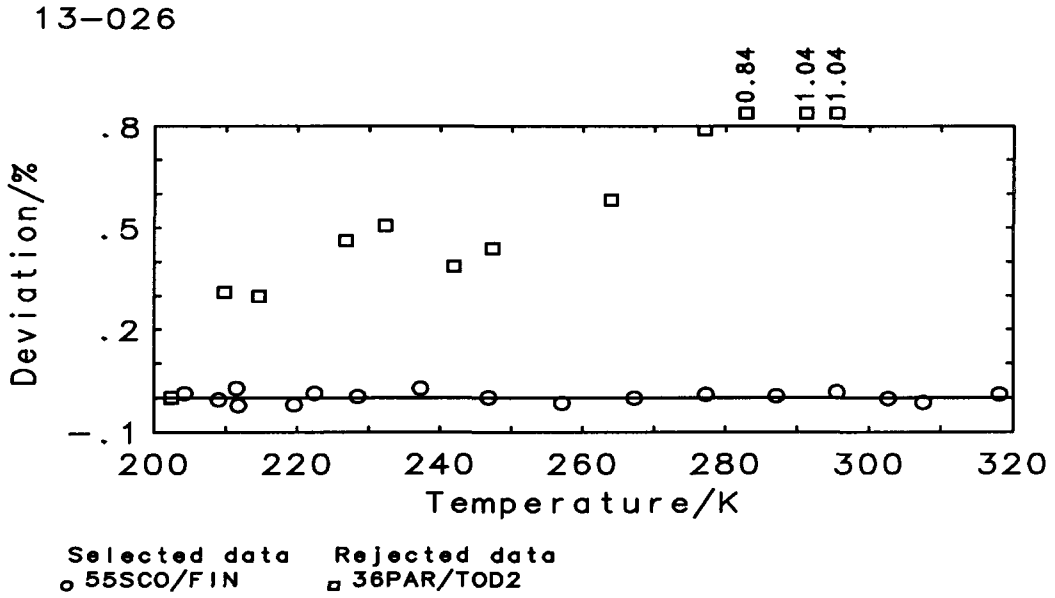
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	18	0.081	3.11–3	0.02	–5.30–7	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
204.3–318.1		2.55879+1	–9.70117	3.76391	–3.43721–1		II

TABLE 13.26.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.827	1.841	1.858	1.877	1.900	1.925	1.953
C_{sat} (J K^{-1}mol^{-1})	153.7	154.9	156.3	158.0	159.9	162.0	164.4
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.983	1.992	2.014	2.048	2.076	2.082	2.119
C_{sat} (J K^{-1}mol^{-1})	166.9	167.7	169.5	172.3	174.7	175.3	178.3
Temp. (K)	320						
c_{sat} (J K^{-1}g^{-1})	2.156						
C_{sat} (J K^{-1}mol^{-1})	181.5						

TABLE 13.26.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	18	0.664	2.65–2	0.13	5.50–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
204.3–318.1	524.00	–3.13792–1	3.48304	1.26417+1	7.06749–3		II



Name: 3,3–Dimethyl–1–butene
Formula: C_6H_{12}

CAS–RN: 558–37–2
Group No.: 13–027
Molar Mass: 84.16

TABLE 13.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38KEN/SHO	165.9–295.9	20	0.70	99.8	estim	C_p	BSIO	25PAR

TABLE 13.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.212	2.80–2	0.15	6.48–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
165.9–295.9		5.38184	1.31325+1	–4.96802	8.45690–1		IV

TABLE 13.27.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1}g^{-1}$)	1.729	1.764	1.798	1.832	1.866	1.900	1.936
C_p ($J K^{-1}mol^{-1}$)	145.5	148.5	151.3	154.2	157.0	159.9	162.9
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	1.973	2.013	2.056	2.101	2.116	2.151	2.204
C_p ($J K^{-1}mol^{-1}$)	166.1	169.4	173.0	176.8	178.1	181.0	185.5
Temp. (K)	298.15	300					
c_p ($J K^{-1}g^{-1}$)	2.251	2.262					
C_p ($J K^{-1}mol^{-1}$)	189.5	190.4					

TABLE 13.27.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.296	3.99–2	0.21	1.42–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
165.9–295.9	490.00	–4.91066	1.73956	1.15768+1	3.46561		IV

Name: 1–Hexene
Formula: C_6H_{12}

CAS–RN: 592–41–6
Group No.: 13–028
Molar Mass: 84.16

TABLE 13.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
57MCC/FIN1	136.2–308.2	23	0.20	99.96	melpt	C_{sat}	BSAO	47HUF
85KAL/WOY	186.6–301.1	31	nosp	99.72	chrom	C_p	BSAO	80KAL/JED

TABLE 13.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57MCC/FIN1	136.2–308.2	23	0.20#	0.166	6.42–3	0.03	3.32–6	–1
				Rejected data				
85KAL/WOY	(1.31–1, 0.67, 8.59–2, 17)							

TABLE 13.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	54	23	0.183	7.06–3	0.04	3.32–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
136.2–308.2		2.30342+1	–6.68116	2.80137	–2.25071–1		II

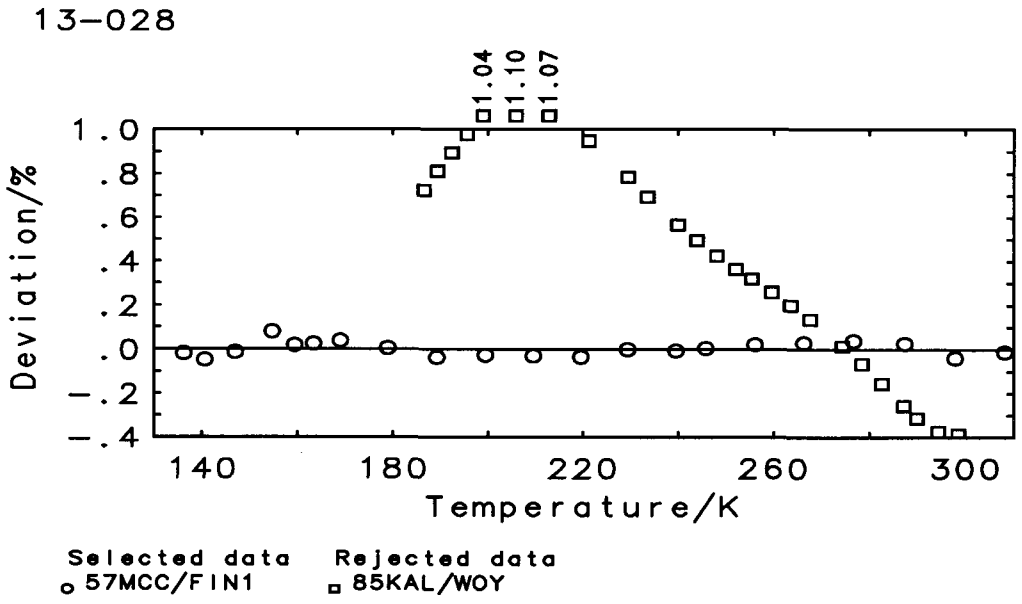
TABLE 13.28.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.833	1.833	1.837	1.844	1.855	1.868	1.885
C_{sat} (J K^{-1}mol^{-1})	154.3	154.3	154.6	155.2	156.1	157.2	158.6
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.904	1.926	1.951	1.978	2.008	2.040	2.073
C_{sat} (J K^{-1}mol^{-1})	160.2	162.1	164.2	166.5	169.0	171.6	174.5
Temp. (K)	273.15	280	290	298.15	300	310	
c_{sat} (J K^{-1}g^{-1})	2.084	2.109	2.147	2.179	2.186	2.227	
C_{sat} (J K^{-1}mol^{-1})	175.4	177.5	180.7	183.3	184.0	187.4	

TABLE 13.28.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	54	23	0.416	1.65–2	0.08	2.05–5	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
136.2–308.2	504.03	2.58690+2	2.29861+1	–5.88457	2.55772+2	8.39159	2.36986+2	II



Name: (Z)–2–Hexene
Formula: C_6H_{12}

CAS–RN: 7688–21–3
Group No.: 13–029
Molar Mass: 84.16

TABLE 13.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90MES/TOD	129.1–314.5	22	0.10	99.963	melpt	C_{sat}	BSAO	47HUF

TABLE 13.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.633	1.25–2	0.06	1.27–5	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
129.1–314.5		2.37227+1	–7.34389	2.86313	–2.20334–1		II

TABLE 13.29.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J $K^{-1}g^{-1}$)	1.831	1.823	1.818	1.818	1.821	1.827	1.837
C_{sat} (J $K^{-1}mol^{-1}$)	154.1	153.4	153.0	153.0	153.2	153.8	154.6
Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J $K^{-1}g^{-1}$)	1.850	1.866	1.885	1.906	1.931	1.958	1.987
C_{sat} (J $K^{-1}mol^{-1}$)	155.7	157.0	158.6	160.4	162.5	164.8	167.2
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J $K^{-1}g^{-1}$)	2.018	2.029	2.052	2.088	2.118	2.125	2.164
C_{sat} (J $K^{-1}mol^{-1}$)	169.9	170.7	172.7	175.7	178.3	178.8	182.1

TABLE 13.29.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	19	0.798	1.58–2	0.08	1.09–5	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
153.3–314.5	512.00	2.35656+2	2.01229+1	–3.58592	2.39437+2	–1.07578+1	2.37094+2	II

Name: 1-Heptene
Formula: C_7H_{14}

CAS-RN: 592-76-7
Group No.: 13-030
Molar Mass: 98.19

TABLE 13.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36PAR/TOD2	151.1–295.1	21	0.50	99.85	melpt	C_p	BSIO	25PAR
57MCC/FIN1	157.1–299.6	22	0.20	99.86	melpt	C_{sat}	BSAO	47HUF

TABLE 13.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57MCC/FIN1	157.1–299.6	22	0.20#	0.110	5.10–3	0.02	6.94–7	0
				Rejected data				
36PAR/TOD2	(1.03–1, 0.43, 4.78–3, –1)							

TABLE 13.30.3. Parameters of regression polynomial

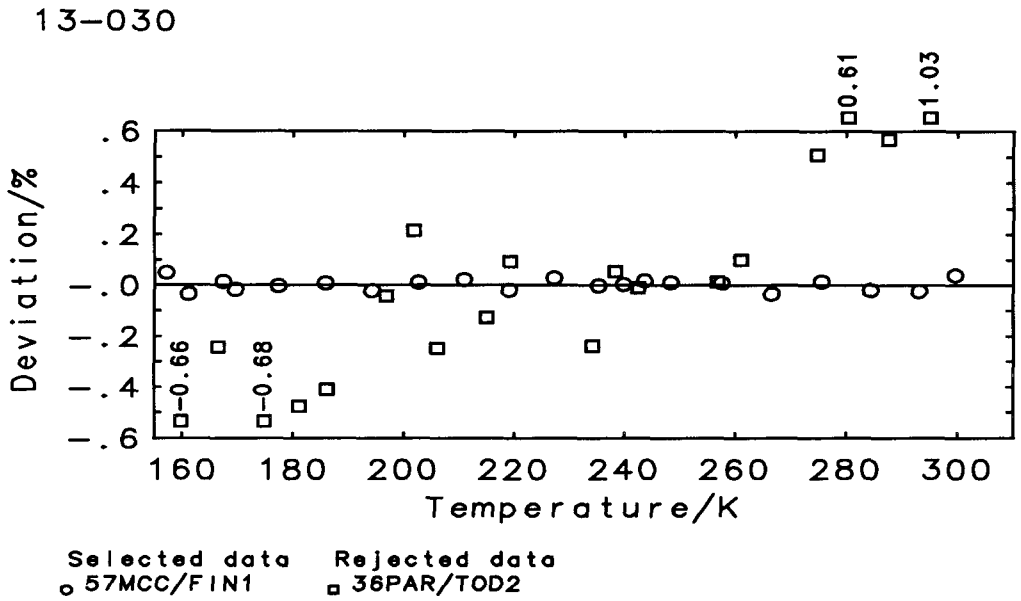
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	43	22	0.122	5.64–3	0.02	6.94–7	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
157.1–299.6		2.95049+1	–1.07928+1	4.41304	–4.18264–1		II

TABLE 13.30.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.848	1.851	1.858	1.868	1.882	1.899	1.919
C_{sat} (J K^{-1}mol^{-1})	181.4	181.7	182.4	183.4	184.8	186.5	188.5
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.942	1.968	1.996	2.026	2.058	2.068	2.092
C_{sat} (J K^{-1}mol^{-1})	190.7	193.2	196.0	198.9	202.1	203.1	205.4
Temp. (K)	290	298.15	300				
c_{sat} (J K^{-1}g^{-1})	2.127	2.157	2.164				
C_{sat} (J K^{-1}mol^{-1})	208.8	211.8	212.4				

TABLE 13.30.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	43	22	0.362	1.67–2	0.07	4.68–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
157.1–299.6	537.30	6.82280+2	7.02369+1	–5.14378+1	6.52620+2	7.78060+1	4.99087+2	II



Name: 1–Octene
Formula: C_8H_{16}

CAS–RN: 111–66–0
Group No.: 13–031
Molar Mass: 112.22

TABLE 13.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
57MCC/FIN1	175.4–308.5	20	0.20	99.94	melpt	C_{sat}	BSAO	47HUF

TABLE 13.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.191	1.01–2	0.04	3.62–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
175.4–308.5		4.53296+1	–2.51051+1	9.75750	–1.06384		II

TABLE 13.31.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.893	1.894	1.900	1.911	1.926	1.946	1.969
C_{sat} (J K^{-1}mol^{-1})	212.4	212.5	213.2	214.4	216.2	218.4	221.0
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.995	2.024	2.055	2.065	2.088	2.122	2.150
C_{sat} (J K^{-1}mol^{-1})	223.9	227.1	230.6	231.8	234.3	238.1	241.3
Temp. (K)	300	310					
c_{sat} (J K^{-1}g^{-1})	2.157	2.192					
C_{sat} (J K^{-1}mol^{-1})	242.0	245.9					

TABLE 13.31.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.609	3.21–2	0.12	7.95–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
175.4–308.5	566.65	2.79268+3	3.22992+2	–3.13143+2	2.65202+3	3.27256+2	1.78737+3	II

Name: 2,4,4–Trimethyl–1–pentene
Formula: C_8H_{16}

CAS–RN: 107–39–1
Group No.: 13–032
Molar Mass: 112.22

TABLE 13.32.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36PAR/TOD2	N	178.4–296.0	15	0.50	99.5	estim	C_p	BSIO	25PAR

36PAR/TOD2 identity of substance was not known exactly (estimated by authors)

TABLE 13.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.177	2.22–2	0.09	2.82–5	1
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
178.4–296.0	1.32041+1	9.41313	–3.44770	6.72476–1	III

TABLE 13.32.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1}g^{-1}$)	1.697	1.723	1.750	1.778	1.807	1.837	1.870
C_p ($J K^{-1}mol^{-1}$)	190.4	193.4	196.4	199.5	202.8	206.2	209.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	1.904	1.941	1.980	1.993	2.022	2.068	2.108
C_p ($J K^{-1}mol^{-1}$)	213.7	217.8	222.2	223.6	226.9	232.0	236.5
Temp. (K)	300						
c_p ($J K^{-1}g^{-1}$)	2.117						
C_p ($J K^{-1}mol^{-1}$)	237.6						

TABLE 13.32.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.194	2.40–2	0.10	4.02–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
178.4–296.0	561.00	–1.65572	7.36809	1.13957+1	9.30166–2		III

Name: 2,4,4–Trimethyl–2–pentene
Formula: C_8H_{16}

CAS–RN: 107–40–4
Group No.: 13–033
Molar Mass: 112.22

TABLE 13.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF1	N	183.0–296.0	8	1.00	not specified		C_p	BSIO	25PAR
36PAR/TOD2	N	170.0–298.6	15	0.50	98.	estim	C_p	BSIO	25PAR

30PAR/HUF1 unspecified isomer; probably mixture of isomers (according to n.m.t.)
36PAR/TOD2 identity of substance was not known exactly (estimated by authors)

TABLE 13.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
36PAR/TOD2	170.0–298.6	15	0.50	0.195	2.64–2	0.10	4.79–5	–5
				Rejected data				
30PAR/HUF1	(6.78–1, 2.68, –6.77–1, –8)							

TABLE 13.33.3. Parameters of regression polynomial

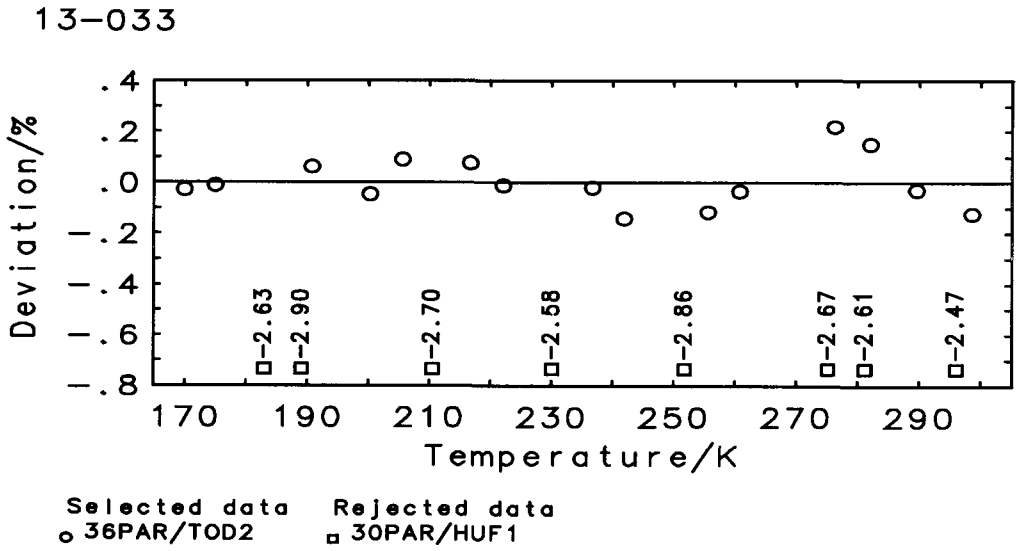
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	15	0.228	3.08–2	0.11	4.79–5	–5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
170.0–298.6		1.00471+1	1.37729+1	–5.04661	8.54456–1		III

TABLE 13.33.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.710	1.739	1.768	1.796	1.825	1.854	1.884
C_p (J K^{-1}mol^{-1})	191.9	195.1	198.4	201.6	204.8	208.0	211.4
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.915	1.948	1.983	2.020	2.032	2.060	2.103
C_p (J K^{-1}mol^{-1})	214.9	218.6	222.5	226.7	228.1	231.2	236.0
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	2.141	2.150					
C_p (J K^{-1}mol^{-1})	240.3	241.3					

TABLE 13.33.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	15	0.340	4.30–2	0.17	1.20–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
170.0–298.6	566.00	–6.19620	4.05142	1.44028+1	2.36910		III



Name: 1–Nonene
Formula: C_9H_{18}

CAS–RN: 124–11–8
Group No.: 13–034
Molar Mass: 126.24

TABLE 13.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90MES/TOD	199.4–380.3	25	0.10	99.979	melpt	C_{sat}	BSAO	47HUF

TABLE 13.34.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.421	1.30–2	0.04	8.09–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
199.4–280.0	6.39017+1	–4.15822+1	1.56093+1	–1.74160	II
280.0–380.3	3.38566+1	–9.39106	4.11242	–3.72925–1	II

TABLE 13.34.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.926	1.929	1.938	1.953	1.972	1.995	2.022
C_{sat} (J K^{-1}mol^{-1})	243.1	243.5	244.7	246.5	248.9	251.9	255.2
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.051	2.061	2.082	2.115	2.142	2.149	2.184
C_{sat} (J K^{-1}mol^{-1})	258.9	260.1	262.9	267.0	270.5	271.3	275.7
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.219	2.256	2.293	2.330	2.368	2.405	2.443
C_{sat} (J K^{-1}mol^{-1})	280.2	284.8	289.4	294.1	298.9	303.6	308.4

TABLE 13.34.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	1.850	5.74–2	0.19	1.66–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
199.4–380.3	593.20	7.06944+2	6.71847+1	–4.22604+1	6.93342+2	3.70320+1	5.94951+2	II

Name: 1–Decene
Formula: $C_{10}H_{20}$

CAS-RN: 872–05–9
Group No.: 13–035
Molar Mass: 140.27

TABLE 13.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57MCC/FIN1	211.4–355.8	19	0.20	99.9	melpt	C_{sat}	BSAO	47HUF

TABLE 13.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.558	3.87–2	0.11	5.14–5	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
211.4–355.8		7.93412+1	–5.17038+1	1.81222+1	–1.89255		II

TABLE 13.35.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.965	1.965	1.972	1.984	2.002	2.025	2.051
C_{sat} (J K^{-1}mol^{-1})	275.7	275.6	276.6	278.3	280.8	284.0	287.7
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	2.060	2.081	2.113	2.141	2.148	2.183	2.220
C_{sat} (J K^{-1}mol^{-1})	289.0	291.9	296.4	300.3	301.2	306.2	311.3
Temp. (K)	330	340	350	360			
c_{sat} (J K^{-1}g^{-1})	2.256	2.291	2.326	2.358			
C_{sat} (J K^{-1}mol^{-1})	316.4	321.4	326.2	330.7			

TABLE 13.35.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	1.014	6.99–2	0.20	2.00–4	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
211.4–355.8	616.70	4.15103+3	4.71647+2	–4.67816+2	4.00277+3	3.42953+2	2.81120+3	II

Name: 1–Undecene
Formula: $C_{11}H_{22}$

CAS-RN: 821–95–4
Group No.: 13–036
Molar Mass: 154.30

TABLE 13.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57MCC/FIN1	227.2–311.4	12	0.20	99.96	melpt	C_{sat}	BSAO	47HUF

TABLE 13.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.403	3.06–2	0.08	3.05–5	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
227.2–311.4	1.44979+2	–1.18448+2	4.19396+1	–4.71375	II

TABLE 13.36.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.997	2.000	2.012	2.030	2.055	2.063	2.083
C_{sat} (J K^{-1}mol^{-1})	308.1	308.6	310.4	313.3	317.0	318.3	321.4

Temp. (K)	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.114	2.140	2.146	2.177
C_{sat} (J K^{-1}mol^{-1})	326.2	330.2	331.1	335.9

TABLE 13.36.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.680	5.13–2	0.14	–2.39–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
227.2–311.4	637.90	5.18289+4	6.86719+3	–7.10688+3	4.78298+4	8.30768+3	2.67726+4	II

Name: 1–Dodecene
Formula: $C_{12}H_{24}$

CAS-RN: 112–41–4
Group No.: 13–037
Molar Mass: 168.32

TABLE 13.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57MCC/FIN1	240.3–305.5	11	0.20	99.92	melpt	C_{sat}	BSAO	47HUF

TABLE 13.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.189	1.57–2	0.04	–7.98–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
240.3–305.5		2.16574+2	–1.88147+2	6.56951+1	–7.40332		II

TABLE 13.37.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	2.029	2.031	2.043	2.063	2.071	2.089	2.118
C_{sat} (J K^{-1}mol^{-1})	341.6	341.9	344.0	347.3	348.6	351.6	356.5
Temp. (K)	298.15	300	310				
c_{sat} (J K^{-1}g^{-1})	2.143	2.149	2.178				
C_{sat} (J K^{-1}mol^{-1})	360.7	361.7	366.6				

TABLE 13.37.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.390	3.24–2	0.08	–2.26–3	–3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
240.3–305.5	657.20	1.74601+5	2.40146+4	–2.47951+4	1.59051+5	3.15074+4	8.34620+4	II

Name: 1–Hexadecene
Formula: $C_{16}H_{32}$

CAS-RN: 629–73–2
Group No.: 13–038
Molar Mass: 224.43

TABLE 13.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
57MCC/FIN1	279.4–303.8	14	0.20	98.7	melpt	C_{sat}	BSAO	47HUF
90MES/TOD	283.9–380.9	32	0.10	99.990	melpt	C_{sat}	BSAO	47HUF

TABLE 13.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57MCC/FIN1	279.4–303.8	14	0.20#	0.805	9.35–2	0.16	–4.92–2	–4
90MES/TOD	283.9–380.9	32	0.10	0.708	4.31–2	0.07	5.48–3	0

TABLE 13.38.3. Parameters of regression polynomial

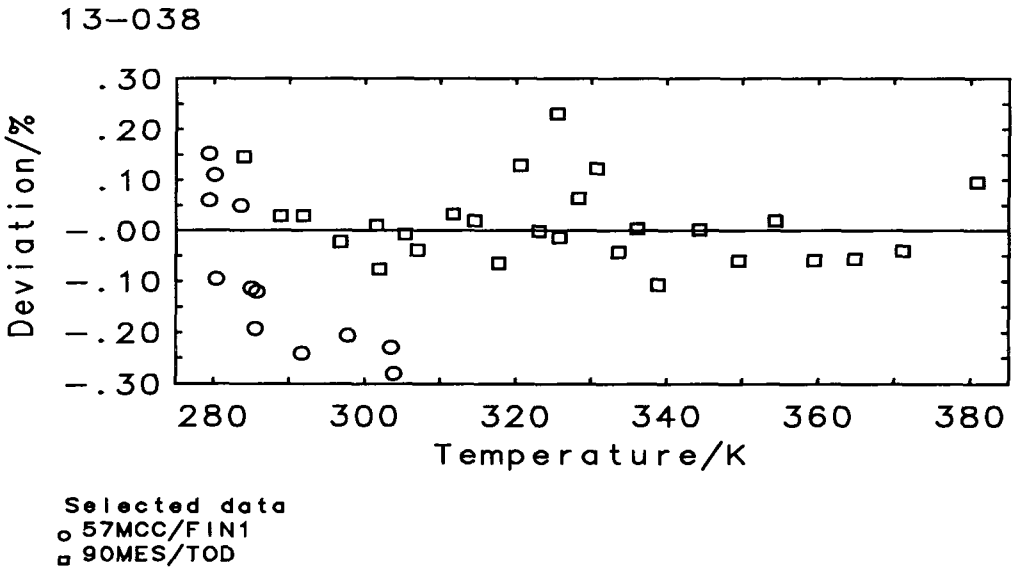
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	46	46	0.773	6.58–2	0.11	–1.12–2	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
279.4–380.9		1.42512+2	–8.35976+1	2.54246+1	–2.29509		II

TABLE 13.38.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	2.126	2.146	2.165	2.170	2.198	2.228	2.261
C_{sat} (J K^{-1}mol^{-1})	477.1	481.6	485.9	487.0	493.2	500.1	507.5
Temp. (K)	340	350	360	370	380		
c_{sat} (J K^{-1}g^{-1})	2.296	2.333	2.370	2.408	2.446		
C_{sat} (J K^{-1}mol^{-1})	515.4	523.6	532.0	540.5	549.1		

TABLE 13.38.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	46	46	0.865	6.96–2	0.12	6.69–3	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
279.4–380.9	719.50	7.40744+3	8.59228+2	–8.41357+2	6.99954+3	9.54338+2	4.66373+3	II



14. Aromatic and Unsaturated Cyclic Hydrocarbons

This family includes 97 compounds, 8 of which were measured at a single temperature only.

A total of 42 compounds of this family were measured at BMB (and later at NIPER) because of their relationships to petroleum, crude tar, and coal (44GUT/SPI, 48HUF/EAT, 48OLI/EAT, 49SCO/GRO, 56FIN/SCO, 57MCC/FIN2, 62SCO/GUT, 65MES/TOD2, 77FIN/MES, 79LEE/HOS, 81LEE/FIN, 82GAM/CAL, 88MES/FIN, 89CHI/HOS, 89CHI/KNI). The data were measured in a high precision adiabatic calorimeter (the reported error of 0.1 to 0.2 % seems to be quite realistic) using high purity samples and were used as a basis for recommendations in all cases. The last two sources included measurements for high-boiling compounds measured using DSC device up to the vicinity of the critical temperature with a reported error of 1 %.

Seven compounds measured at CIUG (67LEB/RAB1, 75LEB/TSV, 78LEB/LEB, 78LEB/TSV, 82LEB/BYK, 88LEB/KUL, 89LEB/SMI) with a reported error of 0.2 to 0.3 % were investigated as monomers which have potential uses in the synthesis of new polymeric materials.

Accurate measurements of five condensed aromatic and bicyclic compounds were carried out at UMMA (70AND/WES, 70GOU/GIR, 70WON/WES, 71WON/WES, 80WON/WES) mainly because of their unusual molecular structure.

Two older measurements for 1,4-dimethylbenzene and ethylbenzene (47COR/GIN, 45SCO/BRI) and two later measurements for two terphenyls (72CHA/BES, 83CHA) were carried out at NBSW.

All the above data have been included in the correlation with the stated uncertainty limits which was warranted by the good reputation of the laboratories and consistency between independent data sources.

Additional data used in the correlation and considered as reliable were obtained from the following laboratories: UOTO (73KIS/SUG, 77HAI/SUG1), UCB (43PIT/SCO, 46PIT/GUT), and RUH (55TAY/KIL, 57PUT/KIL) where three isomers of trimethylbenzene were studied.

When a compound was only measured by a single laboratory, then old measurements from JHUB (31SMI/AND1 1,1-diphenylethylene and 1,1-diphenylethane) and SUC (30HUF/PAR1 tert.butylbenzene and diphenylmethane; 31HUF/PAR 1-isopropyl-4-methylbenzene, 1,2,3,4- and 1,2,3,5-tetramethylbenzene; 32SPA/THO hexamethylbenzene; 33FER/THO 1,2,4,5-tetramethylbenzene and pentamethylbenzene) have been included whose uncertainty limit was about 1 %. Data obtained at PTIL (47KUR, 50KUR) and reported as average heat capacities are considered as only approximative with the error in our judgement exceeding 5 or even 10 % due to the impurities in compounds and the rudimentary experimental technique used.

A variety of compounds from this family were measured at WUSL; the data were presented in a form of an equation and published in two thesis (41SCH, 44EIB). The uncertainty stated by the authors does not seem to be quite realistic and is difficult to estimate what it should be due to the lack of good data from other sources; the expected error can be up to 3 %. In the final selection, the data for four compounds have been examined.

Measurements for 1,3- and 1,4-cyclohexadiene were carried out only at BAF (76GEI/WOL) with a reported error of 3 %. These samples contained considerable amounts of impurities in a form of similar compounds.

This family of compounds contains a large number of chemicals widely used in the chemical industry such as benzene, toluene, styrene, xylenes, and compounds serving as heat transport media in nuclear power stations (such as biphenyl and isopropyl biphenyl). Correspondingly, the frequency of measurements and number of laboratories involved in such measurements are large.

It is surprising that it was difficult to find consistent data for benzene which has been measured most frequently. Measurements from BMB (48OLI/EAT), together with high temperature data from GPI (75RAS/GRI) and MITC (75SAN) have been selected as a basis for the correlation. These data have been supplemented by results obtained at the University St Andrews, Dundee (56DUF/EVE) determined by non-calorimetric (piezometric) method with a reported error below 0.5 %. The piezoelectric data have been selected here due to the absence of reliable calorimetric data in the range between 330 to 353 K. Piezometric data from the same source have also been selected for diphenylmethane as relatively more reliable compared to four available calorimetric sets.

A substantially better situation exists for toluene where two major data sets (BMB measurements 62SCO/GUT, and GITA measurements 66HWA/ZIE, 75HOL/ZIE) agreed to within 0.1 %. At higher temperatures, the data have been supplemented by the measurements from GPI (75RAS/GRI) up to 462 K, (79AND/GRI) up to 373 K and (76SAN/MEL) up to 503 K.

An interesting situation exits in the case of naphthalene where several data sets agree with each other quite well. However, they all differed from the BMB measurements (57MCC/FIN2) which we feel are the most credible source of data. For that reason our recommendations have been based exclusively on the BMB values supplemented for extension of the temperature range by the consistent data generated from an equation given in reference (41SCH).

Different compounds suitable as heat transport media in the power industry were measured using commercial DSC instruments at EREL (83ORO/MRA), at NRLW (58WAL/BRO), and also at MCSL (56MCE/MAL). These measurements were of a routine character and the expected errors are likely to be between 1 and 5 %. An unspecified isomer of isopropylbiphenyl was investigated in fSU laboratories (63VAR/KOP, 64VUK/RAS) and was not fully identified in the literature and the results are subject to considerable uncertainty (over 3 %).

Reliable data for 1,4-dimethylbenzene were obtained at BYUP (79OTT/GOA), and for indane and indene at DCM (61STU/SIN).

Recent extensive measurements on benzene, biphenyl, terphenyl and condensed ring compounds at Laboratoire de Thermodynamique, INPL-ENSIC, Nancy, France (93DUR/AOU) were performed by DSC calorimetry over a wide temperature range. The results show a linear dependence with temperature, however, for those compounds where still other sources of accurate data were available, the slope of the above DSC data was often found to be significantly different. We have expected that the error could be 2–6 % and we included the data only when no other values were available.

Name: Cyclopentene
Formula: C_5H_8

CAS-RN: 142-29-0
Group No.: 14-001
Molar Mass: 68.12

TABLE 14.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48HUF/EAT	140.9–300.8	25	0.20	99.996	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 14.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.184	4.75–3	0.04	4.08–6	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
140.9–300.8		1.86400+1	–9.34139	3.76637	–3.60140–1		II

TABLE 14.1.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.459	1.451	1.448	1.449	1.456	1.467	1.482
C_{sat} (J K^{-1}mol^{-1})	99.41	98.83	98.61	98.74	99.18	99.92	101.0
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.501	1.524	1.550	1.579	1.611	1.646	1.683
C_{sat} (J K^{-1}mol^{-1})	102.2	103.8	105.6	107.6	109.7	112.1	114.6
Temp. (K)	273.15	280	290	298.15	300		
c_{sat} (J K^{-1}g^{-1})	1.695	1.722	1.763	1.797	1.805		
C_{sat} (J K^{-1}mol^{-1})	115.5	117.3	120.1	122.4	123.0		

TABLE 14.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	19	0.409	1.07–2	0.08	1.70–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
163.6–300.8	506.00	3.76498+2	3.57171+1	–2.67450+1	3.75992+2	1.33860	3.29834+2	II

Name: Benzene-d_6
Formula: C_6D_6

CAS-RN: 1076-43-3
Group No.: 14-002
Molar Mass: 84.15

TABLE 14.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
42ZIE/AND		283.5–322.6	9	2.00	99.8	melpt	C_p	BDHO	37STU
62RAB/NIK	N	283.1–303.1	5S	0.30	80.	anal	C_p	BSAO	47SKU

62RAB/NIK substance deuterated to 80 %; results extrapolated to 100 % deuteration

TABLE 14.2.2. Correlated heat capacities

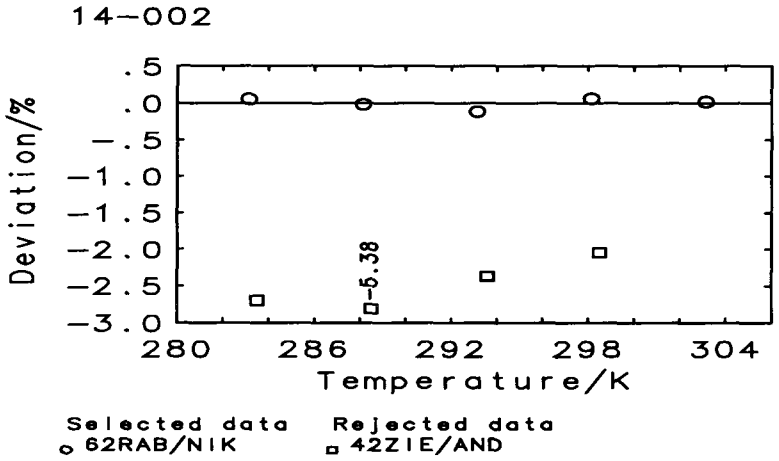
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62RAB/NIK	283.1–303.1	5	0.30	0.215	1.17–2	0.06	1.56–5	1
				Rejected data				
42ZIE/AND	(5.91–1, 3.39, –5.48–1, –4)							

TABLE 14.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	5	0.277	1.52–2	0.08	1.56–5	1
Temp. range K		A_1	A_2				Level of uncertainty
283.1–303.1		1.24486+1	1.97130				III

TABLE 14.2.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.775	1.795	1.811	1.814
C_p (J K^{-1}mol^{-1})	149.4	151.0	152.4	152.7



Name: Benzene
Formula: C_6H_6

CAS-RN: 71–43–2
Group No.: 14–003
Molar Mass: 78.11

TABLE 14.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
19DEJ		297.6–323.1	16	nosp	not specified	C_p	BSIO	19DEJ
21TRE		289.4–331.3	12	nosp	not specified	C_p	BSIO	49WEI
24WIL/DAN		305.0–335.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
25WIL/DAN		293.1–333.1	5S	nosp	not specified	C_p	BSAO	24WIL/DAN
26AND/LYN		293.0–383.0	eqn	nosp	not specified	C_p	DSIO	26AND/LYN
30HUF/PAR1		281.1–300.0	6	1.00	not specified	C_p	BSIO	25PAR
31FIO/GIN	N	328.1–378.1	6S	0.10	not specified	C_{sat}	BSIO	31FIO/GIN
33KOL/UDO	N	287.9	1	nosp	not specified	C_p	BSIT	34KOL/UDO2
37COH/BUI		283.1–295.1	7	nosp	not specified	C_p	BSAO	20COH/MOE
39PHI		301.4	1	nosp	not specified	C_p	BSIO	49WEI
41ZHD		281.4–318.8	3	nosp	not specified	C_p	BSIT	34KOL/UDO2
42ZIE/AND		283.5–322.6	9	2.00	99.99 melpt	C_p	BDHO	37STU
47KUR		290.0–321.8	5	nosp	not specified	C_{avg}	DSIO	47KUR
48OLI/EAT		286.9–336.9	9	0.20	99.967 melpt	C_{sat}	BSAO	43RUE/HUF
48TSC1		295.1	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC5		295.1	1	nosp	not specified	C_p	BSIO	48TSC1
51SIE/CRU	N	293.1	1	nosp	not specified	C_p	not specified	
55STA/TUP		288.4–346.9	13	0.20	not specified	C_p	BSAO	55STA/TUP
56DUF/EVE	N	303.1–353.1	6S	0.50	not specified	C_p	not specified	
60SWI/ZIE	N	316.3–322.1	2	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
62RAB/NIK		283.1–303.1	5S	0.30	not specified	C_p	BSAO	47SKU
65FIN/GRU		300.0	1	0.40	not specified	C_p	BDAO	65FIN/GRU
65KAU/BIT		293.1–349.1	8	1.00	not specified	C_p	FSIO	65KAU/BIT
67PAC		298.1	1	nosp	not specified	C_p	BDHT	79DU/COM
67RAS/GAN		293.1–353.1	4S	0.50	not specified	C_p	BSAO	67RAS/GAN
68REC1	N	298.0–313.0	eqn	nosp	not specified	C_p	BSAO	68REC1
71DES/BHA		298.1–318.1	3S	1.00	not specified	C_p	BSIO	56MUR/VAN
71KHA/SUB	N	298.1–313.1	2	nosp	not specified	C_p	BSIO	64MOE/THO
74RAJ/SUB		298.1–323.1	3	0.30	not specified	C_p	BSIO	64MOE/THO
75RAS/GRI	N	305.1–463.1	9	nosp	not specified	C_p	BDAO	75RAS/GRI
75SAN	N	433.1–493.1	6S	1.00	not specified	C_p	FSIO	75SAN
76FOR/BEN2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
77WIL/GRO		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
78GRO/WIL		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
81ATA/ELS		293.1	1	2.50	not specified	C_p	BDHO	81ATA/ELS
82GRO/ING		298.1	1	nosp	98.5 melpt	C_p	FSIT	71PIC/LED
82TAN		293.1–303.1	3S	0.30	99.99 melpt	C_p	FSIT	71PIC/LED
82WIL/FAR		298.1	1	nosp	98.5 melpt	C_p	FSIT	71PIC/LED
83GOR/SIM	N	283.8–348.5	12	0.25	99.9 anal	C_p	FSIO	83GOR/SIM
85OGA		298.1	1	0.10	not specified	C_p	FSIO	85OGA
85TAN		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
86NAZ/BAS1		322.0–351.1	2	2.00	not specified	C_p	BDHO	86NAZ/BAS1
87KAL/KOH		293.1–313.1	2	nosp	not specified	C_p	FSIT	71PIC/LED
87TAN		293.1–303.1	3	nosp	not specified	C_p	FSIT	71PIC/LED

TABLE 14.3.1. Experimental heat capacities (continued)

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88SHI/OGA1	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA
89LAI/ROD	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
89PRA/RAJ	318.1–333.1	4	3.00	not specified		C_p	BDHT	89PRA/RAJ
90YAM/OGA	298.1	1	nosp	99.97	chrom	C_p	FSIO	85OGA
91CZA	298.5	1	2.00	not specified		C_p	BSIO	79CZA
91GRO/ROU	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
91TAN/ADA	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
91WIL/JIM	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
92MIY/TAM	298.1	1	nosp	99.99	chrom	C_p	FSIO	85OGA
93DUR/AOU	303.0–347.0	23	nosp	not specified		C_p	BDCT	86MER/BEN

31FIO/GIN water content below 0.01 %; data calculated using procedure by 85WIL/CHA
33KOL/UDO same datum in 34KOL/UDO2
51SIE/CRU heat of mixing calorimeter used
56DUF/EVE measured by a non–calorimetric method (piezo–thermometric)
60SWI/ZIE average values in temperature ranges 294–339 K and 294–350 K
68REC1 same data in 68REC2
71KHA/SUB reproducibility given as 0.3 %
75RAS/GRI data above 343 K measured at superambient pressures up to 1.33 MPa
75SAN same data in 76SAN/MEL; C_p at saturation curve extrapolated from high pressure measurements
83GOR/SIM same data in 82GOR/GRI

TABLE 14.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48OLI/EAT	286.9–336.9	9	0.20	0.361	1.19–2	0.07	3.56–3	3
56DUF/EVE	303.1–353.1	6	0.50	0.527	4.46–2	0.26	6.12–3	0
65FIN/GRU	300.0	1	0.40	0.218	1.43–2	0.09	1.43–2	1
71KHA/SUB	298.1–313.1	2	0.50#	0.384	3.21–2	0.19	–2.20–2	–1
75RAS/GRI	305.1–463.1	9	0.80#	1.239	2.06–1	0.99	–5.40–2	–3
75SAN	433.1–493.1	6	1.00	0.580	1.34–1	0.58	8.40–2	4
76FOR/BEN2	298.1	1	0.30	0.315	1.54–2	0.09	–1.54–2	–1
77WIL/GRO	298.1	1	0.30	0.709	3.47–2	0.21	–3.47–2	–1
78GRO/WIL	298.1	1	0.30	0.684	3.35–2	0.21	–3.35–2	–1
82GRO/ING	298.1	1	0.50#	0.248	2.03–2	0.12	–2.03–2	–1
82TAN	293.1–303.1	3	0.30	0.433	2.12–2	0.13	–2.11–2	–3
85OGA	298.1	1	0.10	1.261	2.06–2	0.13	2.06–2	1
85TAN	298.1	1	0.30	0.414	2.03–2	0.12	–2.03–2	–1
87TAN	293.1–303.1	3	0.50#	0.322	2.63–2	0.16	–2.61–2	–3
89LAI/ROD	298.1	1	0.50#	0.396	3.23–2	0.20	–3.23–2	–1
91GRO/ROU	298.1	1	0.50#	0.366	2.99–2	0.18	–2.99–2	–1
91TAN/ADA	298.1	1	0.50#	0.307	2.51–2	0.15	–2.51–2	–1
92MIY/TAM	298.1	1	0.50#	0.076	6.20–3	0.04	6.20–3	1

TABLE 14.3.2. Correlated heat capacities (continued)

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Rejected data				
19DEJ	(2.74–1, 1.61, 2.49–1, 16)			21TRE	(1.61–1, 0.96, 4.26–2, 4)			
24WIL/DAN	(2.90–1, 1.68, 3.93–2, 1)			25WIL/DAN	(3.38–1, 1.94, 1.60–3, –1)			
26AND/LYN	(3.30–1, 1.93, –1.33–3, 1)			30HUF/PAR1	(1.25–1, 0.77, –1.24–1, –3)			
31FIO/GIN	(1.32–1, 0.74, 1.30–1, 6)			33KOL/UDO	(3.05–1, 1.93, –3.05–1, –1)			
37COH/BUI	(2.31–1, 1.45, –2.30–1, –5)			39PHI	(7.37–2, 0.45, –7.37–2, –1)			
41ZHD	(3.53–2, 0.21, 2.42–2, 1)			42ZIE/AND	(1.62–1, 0.97, –6.86–2, –6)			
47KUR	(2.70–1, 1.70, –1.78–1, –3)			48TSC1	(2.31–1, 1.44, –2.31–1, –1)			
48TSC5	(1.53–1, 0.95, –1.53–1, –1)			51SIE/CRU	(2.09–1, 1.30, –2.09–1, –1)			
55STA/TUP	(1.30–1, 0.77, –1.19–1, –13)			60SWI/ZIE	(5.26–1, 3.23, –3.20–1, 0)			
62RAB/NIK	(1.10–1, 0.68, –1.10–1, –4)			65KAU/BIT	(3.54–1, 2.00, 1.05–1, 0)			
67PAC	(6.20–1, 3.94, –6.20–1, –1)			67RAS/GAN	(7.62–2, 0.44, 5.51–2, 2)			
68REC1	(5.90–2, 0.36, –5.88–2, –5)			71DES/BHA	(1.95–1, 1.19, –1.95–1, –3)			
74RAJ/SUB	(6.84–2, 0.41, –6.04–2, –3)			81ATA/ELS	(1.56–1, 0.97, –1.56–1, –1)			
82WIL/FAR	(3.47–2, 0.21, –3.47–2, –1)			83GOR/SIM	(8.78–2, 0.51, 7.55–2, 10)			
86NAZ/BAS1	(1.76–1, 1.01, –7.54–3, 0)			87KAL/KOH	(5.46–2, 0.33, –5.09–2, –2)			
88SHI/OGA1	(1.51–1, 0.93, –1.51–1, –1)			89PRA/RAJ	(4.57–1, 2.73, –4.39–1, –4)			
90YAM/OGA	(8.16–2, 0.50, –8.16–2, –1)			91CZA	(5.34–3, 0.03, –5.34–3, –1)			
91WIL/JIM	(3.47–2, 0.21, –3.47–2, –1)			93DUR/AOU	(2.78–1, 1.61, 2.76–1, 23)			

TABLE 14.3.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	226	49	0.726	1.08–1	0.52	–5.49–3	–8
C_{sat}	226	49	0.717	1.05–1	0.51	–5.70–3	–8

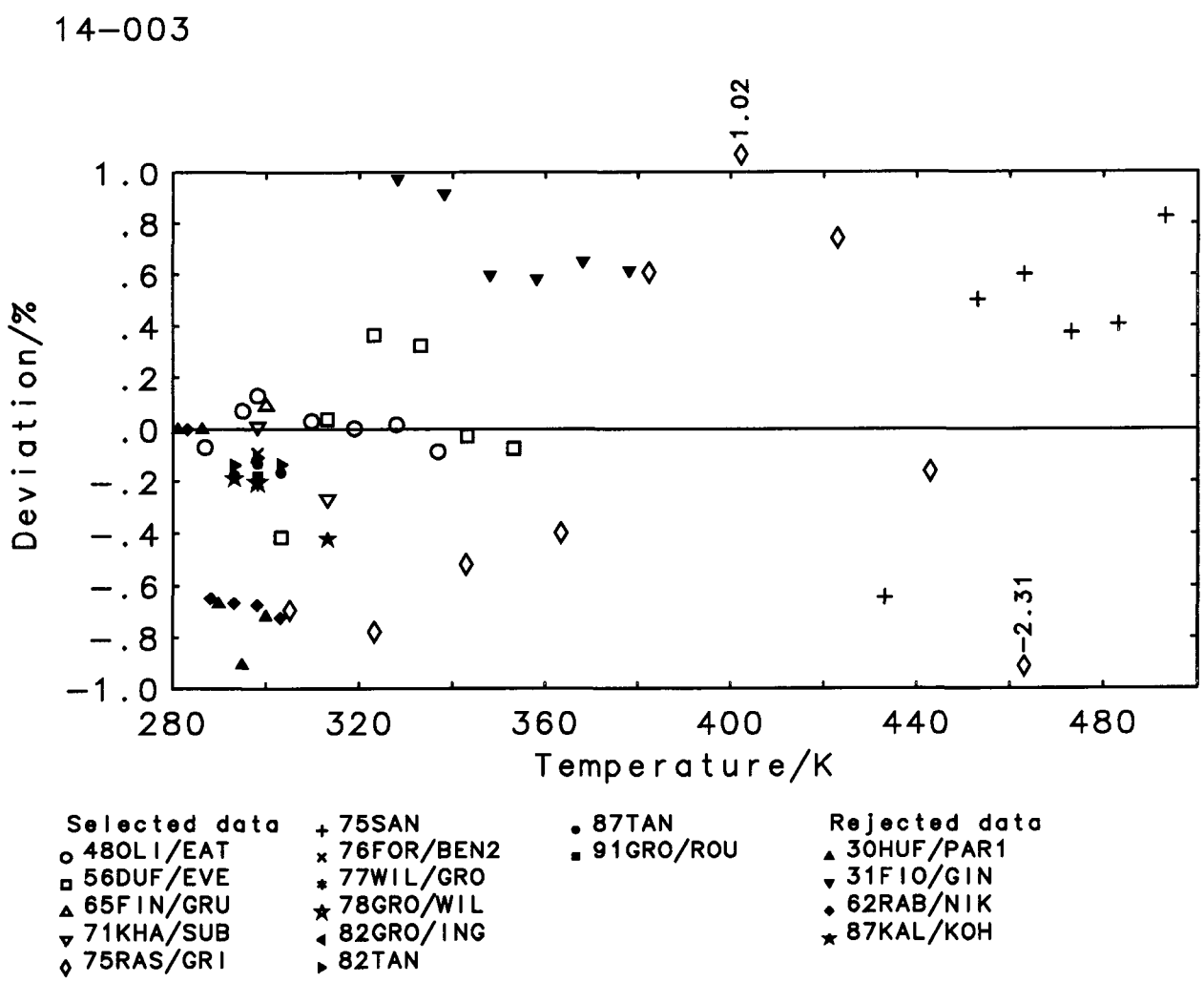
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
286.9–353.0	5.18892+1	–3.65279+1	1.16595+1	–1.14259	III
353.0–493.1	–5.36489+1	5.31646+1	–1.37492+1	1.25671	IV
286.9–353.0	4.90773+1	–3.39839+1	1.09030+1	–1.06896	III
353.0–493.1	–4.38720+1	4.50098+1	–1.14748+1	1.04415	IV

TABLE 14.3.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	1.719	1.740	1.745	1.773	1.804	1.837	1.870
C_p ($J\,K^{-1}mol^{-1}$)	134.3	135.9	136.3	138.5	141.0	143.5	146.1
c_{sat} ($J\,K^{-1}g^{-1}$)	1.719	1.740	1.745	1.773	1.804	1.836	1.869
C_{sat} ($J\,K^{-1}mol^{-1}$)	134.3	135.9	136.3	138.5	140.9	143.4	146.0
Temp. (K)	350	360	370	380	390	400	410
c_p ($J\,K^{-1}g^{-1}$)	1.903	1.936	1.968	2.001	2.035	2.071	2.109
C_p ($J\,K^{-1}mol^{-1}$)	148.7	151.2	153.7	156.3	158.9	161.7	164.8
c_{sat} ($J\,K^{-1}g^{-1}$)	1.901	1.934	1.965	1.997	2.030	2.065	2.101
C_{sat} ($J\,K^{-1}mol^{-1}$)	148.5	151.0	153.5	156.0	158.6	161.3	164.1
Temp. (K)	420	430	440	450	460	470	480
c_p ($J\,K^{-1}g^{-1}$)	2.152	2.198	2.250	2.309	2.374	2.446	2.527
C_p ($J\,K^{-1}mol^{-1}$)	168.1	171.7	175.8	180.3	185.4	191.1	197.4
c_{sat} ($J\,K^{-1}g^{-1}$)	2.141	2.184	2.231	2.284	2.342	2.406	2.477
C_{sat} ($J\,K^{-1}mol^{-1}$)	167.2	170.6	174.3	178.4	182.9	187.9	193.5
Temp. (K)	490						
c_p ($J\,K^{-1}g^{-1}$)	2.617						
C_p ($J\,K^{-1}mol^{-1}$)	204.5						
c_{sat} ($J\,K^{-1}g^{-1}$)	2.556						
C_{sat} ($J\,K^{-1}mol^{-1}$)	199.6						

TABLE 14.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	226	49	0.795	1.11–1	0.53	–9.05–3	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
286.9–493.1	562.16	–3.06796	3.49088–1	9.70407	6.74068		IV



Name: 1,3–Cyclohexadiene
Formula: C_6H_8

CAS-RN: 592–57–4
Group No.: 14–004
Molar Mass: 80.13

TABLE 14.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76GIE/WOL	N	170.0–300.0	14S	3.00	89.4	chrom	C_p	BSIO	76GIE/WOL
89STE/CHI3		298.1	1	1.00	99.95	chrom	C_p	BDHT	89KNI/ARC

76GIE/WOL sample contained 9 % 1,4–Cyclohexadiene, 0.8 % Benzene and 0.8 % Cyclohexene

TABLE 14.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76GIE/WOL	170.0–300.0	14	3.00	0.230	1.17–1	0.69	4.92–2	0
89STE/CHI3	298.1	1	1.00	0.432	7.35–2	0.43	–7.35–2	–1

TABLE 14.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.278	1.29–1	0.76	4.10–2	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
170.0–300.0		1.29885+1	–4.76553–1	6.19334–1			V

TABLE 14.4.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.45	1.47	1.49	1.51	1.53	1.55	1.57
C_p (J K^{-1}mol^{-1})	116	118	119	121	122	124	126
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.60	1.63	1.65	1.68	1.69	1.71	1.74
C_p (J K^{-1}mol^{-1})	128	130	133	135	136	137	140
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.77	1.78					
C_p (J K^{-1}mol^{-1})	142	142					

TABLE 14.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.605	1.05–1	0.62	–1.77–2	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
170.0–300.0	560.00	7.18648	8.35630	4.12380	1.54511		V

Name: 1,4–Cyclohexadiene
Formula: C_6H_8

CAS-RN: 628–41–1
Group No.: 14–005
Molar Mass: 80.13

TABLE 14.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76GIE/WOL	N	230.0–300.0	8S	3.00	96.7	chrom	C_p	BSIO	76GIE/WOL
89STE/CHI3		298.1	1	1.00	99.9	chrom	C_p	BDHT	89KNI/ARC

76GIE/WOL sample contained 3.3 % Cyclohexene

TABLE 14.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76GIE/WOL	230.0–300.0	8	3.00	0.324	1.70–1	0.97	7.71–2	0
89STE/CHI3	298.1	1	1.00	0.381	6.52–2	0.38	–6.52–2	–1

TABLE 14.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.405	1.98–1	1.13	6.13–2	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
230.0–300.0		9.54238	3.54110	–3.30214–1			V

TABLE 14.5.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	1.65	1.67	1.69	1.71	1.73	1.74	1.75
C_p ($J K^{-1} mol^{-1}$)	133	134	136	137	139	139	140
Temp. (K)	290	298.15	300				
c_p ($J K^{-1} g^{-1}$)	1.77	1.78	1.78				
C_p ($J K^{-1} mol^{-1}$)	142	143	143				

TABLE 14.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	1.015	1.78–1	1.04	–4.14–2	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
230.0–300.0	567.60	5.61346+1	2.41382+1	–8.64491	3.26359+1		V

Name: Cyclohexene
Formula: C_6H_{10}

CAS-RN: 110–83–8
Group No.: 14–006
Molar Mass: 82.15

TABLE 14.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30PAR/HUF1	175.2–293.2	12	1.00	not specified		C_p	BSIO	25PAR
48HUF/EAT	178.8–300.6	19	0.20	99.997	melpt	C_{sat}	BSAO	43RUE/HUF
77HAI/SUG1	171.2–293.4	42	nosp	99.96	melpt	C_{sat}	BSAO	65SUG/SEK
88KAL/WOY	183.0–298.1	26	nosp	not specified		C_p	BSAO	80KAL/JED

TABLE 14.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48HUF/EAT	178.8–300.6	19	0.20#	1.703	5.39–2	0.34	5.34–2	19
77HAI/SUG1	171.2–293.4	42	0.20#	0.830	2.66–2	0.17	–2.39–2	–41
				Rejected data				
30PAR/HUF1	(1.33–1, 0.84, –1.23–1, –12)			88KAL/WOY	(2.19–1, 1.32, 1.99–1, 26)			

TABLE 14.6.3. Parameters of regression polynomial

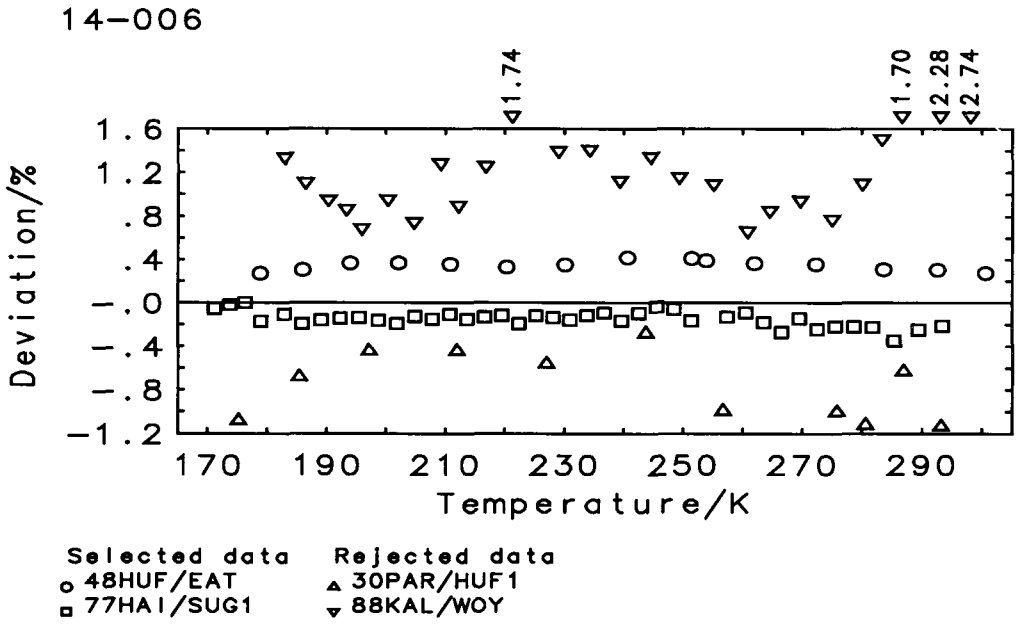
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	99	61	1.214	3.86–2	0.24	1.75–4	–2 2
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
171.2–300.6	1.66241+1	–5.46846	2.71146	–2.46606–1			II

TABLE 14.6.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.412	1.430	1.451	1.474	1.499	1.527	1.558
C_{sat} (J K^{-1}mol^{-1})	116.0	117.5	119.2	121.1	123.2	125.5	128.0
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.590	1.624	1.660	1.698	1.710	1.737	1.777
C_{sat} (J K^{-1}mol^{-1})	130.6	133.4	136.4	139.5	140.4	142.7	146.0
Temp. (K)	298.15	300					
c_{sat} (J K^{-1}g^{-1})	1.810	1.818					
C_{sat} (J K^{-1}mol^{-1})	148.7	149.4					

TABLE 14.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	99	61	1.407	4.44–2	0.28	–2.89–4	–9
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
171.2–300.6	560.50	3.29996–1	5.96405	5.45636	4.56474–3		III



Name: 1–Methylcyclopentene
Formula: C_6H_{10}

CAS–RN: 693–89–0
Group No.: 14–007
Molar Mass: 82.15

TABLE 14.7.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC/PEA	298.15	1.864	1.50	99.	chrom	C_p	BSIO	80FUC

Name: 3–Methylcyclopentene
Formula: C_6H_{10}

CAS–RN: 1120–62–3
Group No.: 14–008
Molar Mass: 82.15

TABLE 14.8.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC/PEA	298.15	1.854	1.50	99.	chrom	C_p	BSIO	80FUC

Name: Bicyclo[2.2.1]hepta–2,5–diene
Formula: C_7H_8

CAS-RN: 121–46–0
Group No.: 14–009
Molar Mass: 92.14

TABLE 14.9.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73HAL/SMI	297.15	1.260	nosp	99.9	chrom	C_p	BDHT	71DU/COM

Name: 1,3,5–Cycloheptatriene
Formula: C_7H_8

CAS-RN: 544–25–2
Group No.: 14–010
Molar Mass: 92.14

TABLE 14.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56FIN/SCO	201.5–312.2	19	0.20	99.986	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 14.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.104	3.81–3	0.02	1.91–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
201.5–312.2		1.68356+1	–2.20006	1.26682	–7.38067–2		II

TABLE 14.10.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.526	1.545	1.565	1.586	1.609	1.633	1.659
C_{sat} (J K^{-1}mol^{-1})	140.6	142.3	144.2	146.2	148.3	150.5	152.8
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.685	1.694	1.713	1.742	1.767	1.773	1.804
C_{sat} (J K^{-1}mol^{-1})	155.3	156.1	157.9	160.5	162.8	163.3	166.2

TABLE 14.10.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.256	9.38–3	0.05	7.53–6	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
201.5–312.2	609.60	–2.31325	4.24880	9.55177	3.14862–1		II

Name: Methylbenzene
Formula: C_7H_8

CAS-RN: 108–88–3
Group No.: 14–011
Molar Mass: 92.14

TABLE 14.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON		304.8–341.3	7S	nosp	not specified	C_{avg}	DSIO	*81VON
*86SCH		309.3–329.0	11S	nosp	not specified	C_{avg}	DSIO	*86SCH
07BAT	N	181.1–248.1	6	nosp	not specified	C_p	BSIO	07BAT
24WIL/DAN		305.0–348.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
25WIL/DAN		293.1–333.1	5S	nosp	not specified	C_p	BSAO	24WIL/DAN
29KEL5	N	183.8–284.4	11	nosp	not specified	C_p	BSIO	29KEL1
30SOU/AND	N	183.8–244.8	7	0.50	not specified	C_p	BSAO	30SOU/AND
31SMI/AND1		184.4–298.5	9	nosp	not specified	C_p	DSIO	26AND/LYN
35AOY/KAN		195.2–227.8	2	nosp	not specified	C_p	BSAO	35AOY/KAN
37VOL		298.1	1	nosp	not specified	C_p	BSIO	37VOL
41ZHD		278.5–320.4	3	nosp	not specified	C_p	BSIT	34KOL/UDO2
47KUR		241.9–310.5	4	nosp	not specified	C_{avg}	DSIO	47KUR
48TSC1		295.1	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC5		295.1	1	nosp	not specified	C_p	BSIO	48TSC1
56SCH/GOT		270.0–292.5	10	2.00	not specified	C_p	BSAO	33SOU/BRI
58SWI/ZIE2	N	323.9–333.2	2	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
62SCO/GUT		183.2–371.0	23	0.20	99.999 melpt	C_{sat}	BSAO	47HUF
66HWA/ZIE		180.9–304.4	34	nosp	99.99 melpt	C_p	BSAO	45SCO/MEY
67RAS/GAN		293.1–373.1	5S	0.50	not specified	C_p	BSAO	67RAS/GAN
71DES/BHA		298.1–318.1	3S	1.00	not specified	C_p	BSIO	56MUR/VAN
73AKH/EKS		298.1	1	0.20	not specified	C_p	FSIO	59RIB/EGO
74RAJ/SUB		298.1–323.1	3	0.30	not specified	C_p	BSIO	64MOE/THO
75HOL/ZIE		162.0–312.0	eqn	0.20	not specified	C_p	BSAO	45SCO/MEY
75PED/KAY		300.6–347.3	19	nosp	not specified	C_p	BSIO	75PED/KAY
75RAS/GRI	N	303.0–462.7	9	1.00	not specified	C_p	BDAO	75RAS/GRI
76FOR/BEN1		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
76SAN/MEL	N	393.1–503.1	8S	1.00	not specified	C_p	FSIO	75SAN
77FOR/BEN		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
77WIL/GRO		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
79AND/GRI	N	293.1–373.3	9	0.50	not specified	C_p	BSAO	67RAS/GAN
80NEF/FIL		300.0–520.0	12S	nosp	not specified	C_{sat}	BDHO	84FIL/LAU
81ATA/ELS		293.1	1	2.50	not specified	C_p	BDHO	81ATA/ELS
82GRO/ING		298.1	1	0.30	99.5 estim	C_p	FSIT	71PIC/LED
82WIL/FAR		298.1	1	0.30	99.5 estim	C_p	FSIT	71PIC/LED
84STE/OLS		266.1–318.1	11S	nosp	99.5 melpt	C_p	BDHT	69PER/COM
85COS/PAT6		298.2	1	nosp	99. anal	C_p	FSIT	71PIC/LED
86ROU/GRO		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
87OKH/RAZ		181.4–380.4	15	0.30	not specified	C_{sat}	BDAO	87OKH/RAZ
88SHI/OGA1		298.1	1	nosp	99.9 chrom	C_p	FSIO	85OGA
89PRA/RAJ		318.1–333.1	4	3.00	not specified	C_p	BDHT	89PRA/RAJ
90RAO/RAJ		318.1–333.1	4	4.00	not specified	C_p	BDHT	89PRA/RAJ
91COB/GAR		298.1–368.1	4	nosp	not specified	C_p	BDCT	83ROU/ROU
91TAN/ADA		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED

07BAT same data in 08BAT
29KEL5 high sample purity
30SOU/AND high sample purity
58SWI/ZIE2 average values in temperature ranges 294–354 K and 294–372 K
75RAS/GRI data above 364 K measured at superambient pressures up to 0.72 MPa
76SAN/MEL C_p at saturation curve extrapolated from high pressure measurements
79AND/GRI grade: pure

TABLE 14.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62SCO/GUT	183.2–371.0	23	0.20	0.462	1.83–2	0.09	2.00–3	2
66HWA/ZIE	180.9–304.5	34	0.20#	0.426	1.50–2	0.09	2.43–3	–2
75HOL/ZIE	162.0–312.0	31	0.20	0.277	1.03–2	0.06	–6.72–3	–22
75RAS/GRI	303.0–462.7	9	1.00	0.624	1.50–1	0.62	–2.18–2	1
76FOR/BEN1	298.1	1	0.30	0.220	1.25–2	0.07	–1.25–2	–1
76SAN/MEL	393.1–503.1	8	1.00	0.427	1.12–1	0.43	7.29–2	6
77FOR/BEN	298.1	1	0.50#	0.062	5.87–3	0.03	–5.87–3	–1
77WIL/GRO	298.1	1	0.30	0.403	2.28–2	0.12	–2.28–2	–1
79AND/GRI	293.1–373.3	9	0.50	0.811	8.02–2	0.41	7.36–2	9
82GRO/ING	298.1	1	0.30	0.254	1.44–2	0.08	–1.44–2	–1
82WIL/FAR	298.1	1	0.30	0.043	2.42–3	0.01	2.42–3	1
86ROU/GRO	298.1	1	0.50#	0.063	5.99–3	0.03	–5.99–3	–1
91COB/GAR	298.1–368.1	4	0.50#	0.215	2.08–2	0.11	–1.65–2	–3
91TAN/ADA	298.1	1	0.50#	0.178	1.68–2	0.09	–1.68–2	–1
91WIL/JIM	298.1	1	0.50#	0.114	1.08–2	0.06	–1.08–2	–1
				Rejected data				
*81VON	(3.03–1, 1.52, 2.66–1, 5)			*86SCH	(3.70–1, 1.83, 3.62–1, 11)			
07BAT	(1.08–1, 0.63, 9.06–2, 6)			24WIL/DAN	(5.43–1, 2.82, –5.41–1, –5)			
25WIL/DAN	(5.52–1, 2.93, –5.52–1, –5)			29KEL5	(2.11–1, 1.24, –1.81–1, –11)			
30SOU/AND	(1.95–1, 1.17, –1.80–1, –7)			31SMI/AND1	(3.34–1, 1.92, –1.61–1, –5)			
35AOY/KAN	(1.54–1, 0.90, 1.27–1, 2)			37VOL	(7.81–2, 0.41, –7.81–2, –1)			
41ZHD	(2.61–1, 1.38, 1.88–2, 1)			47KUR	(6.39–1, 3.84, –2.84–1, 0)			
48TSC1	(2.59–1, 1.36, 2.59–1, 1)			48TSC5	(4.90–1, 2.54, 4.90–1, 1)			
56SCH/GOT	(4.74–1, 2.52, 4.71–1, 10)			58SWI/ZIE2	(2.87–1, 1.42, 2.87–1, 2)			
67RAS/GAN	(2.24–1, 1.07, –1.15–1, –1)			71DES/BHA	(1.89–1, 0.98, –1.72–1, –3)			
73AKH/EKS	(4.07–2, 0.21, 4.07–2, 1)			74RAJ/SUB	(1.43–1, 0.72, 9.72–2, 1)			
75PED/KAY	(1.06–1, 0.53, 5.47–2, 4)			80NEF/FIL	(4.93–1, 1.85, –3.18–1, –9)			
81ATA/ELS	(2.96–2, 0.16, 2.96–2, 1)			84STE/OLS	(1.67–1, 0.87, 1.55–1, 11)			
85COS/PAT6	(1.87–1, 0.98, 1.87–1, 1)			87OKH/RAZ	(1.53–1, 0.77, 1.02–1, 10)			
88SHI/OGA1	(1.41–1, 0.75, –1.41–1, –1)			89PRA/RAJ	(3.29–1, 1.62, 3.25–1, 4)			
90RAO/RAJ	(7.97–1, 4.21, –7.81–1, –4)							

TABLE 14.11.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	291	126	0.455	5.64–2	0.24	6.49–3	–15
C_{sat}	291	126	0.459	5.67–2	0.24	6.58–3	–15

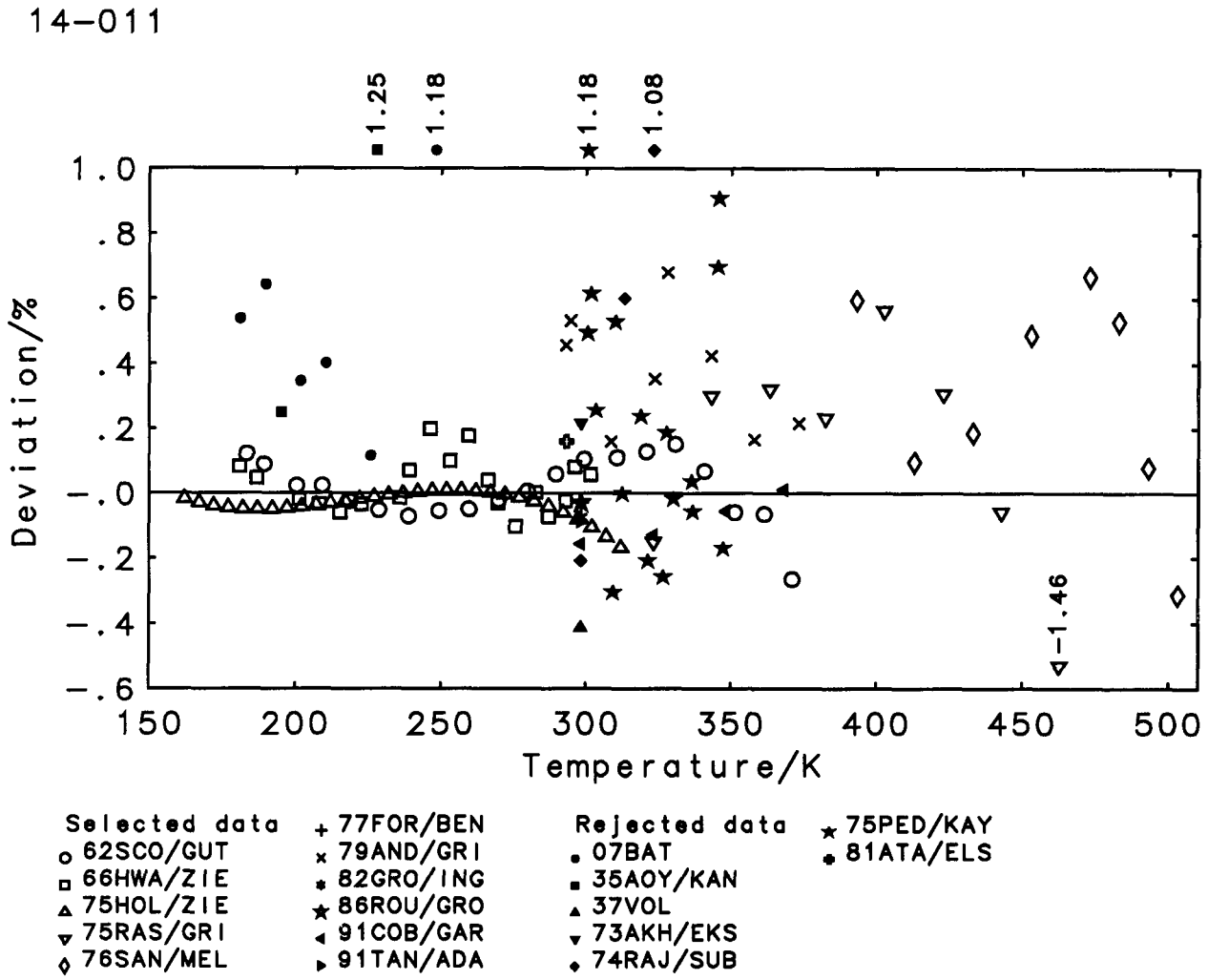
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
162.0–300.0	2.19038+1	–7.86604	3.13678	–2.80597–1	II
300.0–400.0	1.61637+1	–2.12595	1.22342	–6.80006–2	III
400.0–503.1	–9.49111+1	8.11801+1	–1.96031+1	1.66754	IV
162.0–300.0	2.19306+1	–7.90144	3.15203	–2.82743–1	II
300.0–400.0	1.68655+1	–2.83637	1.46367	–9.51468–2	III
400.0–503.1	–8.43158+1	7.30496+1	–1.75078+1	1.48581	IV

TABLE 14.11.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1} g^{-1}$)	1.463	1.468	1.476	1.487	1.500	1.515	1.533
C_p ($J K^{-1} mol^{-1}$)	134.8	135.3	136.0	137.0	138.2	139.6	141.3
c_{sat} ($J K^{-1} g^{-1}$)	1.464	1.468	1.476	1.487	1.500	1.515	1.533
C_{sat} ($J K^{-1} mol^{-1}$)	134.8	135.3	136.0	137.0	138.2	139.6	141.3
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	1.553	1.575	1.599	1.625	1.634	1.652	1.681
C_p ($J K^{-1} mol^{-1}$)	143.1	145.2	147.4	149.7	150.5	152.3	154.9
c_{sat} ($J K^{-1} g^{-1}$)	1.553	1.575	1.599	1.625	1.634	1.652	1.681
C_{sat} ($J K^{-1} mol^{-1}$)	143.1	145.2	147.4	149.7	150.5	152.3	154.9
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.705	1.711	1.742	1.774	1.807	1.841	1.876
C_p ($J K^{-1} mol^{-1}$)	157.1	157.6	160.5	163.5	166.5	169.7	172.9
c_{sat} ($J K^{-1} g^{-1}$)	1.705	1.711	1.742	1.774	1.807	1.841	1.876
C_{sat} ($J K^{-1} mol^{-1}$)	157.1	157.6	160.5	163.5	166.5	169.6	172.8
Temp. (K)	360	370	380	390	400	410	420
c_p ($J K^{-1} g^{-1}$)	1.912	1.949	1.987	2.026	2.065	2.105	2.147
C_p ($J K^{-1} mol^{-1}$)	176.2	179.6	183.1	186.6	190.3	194.0	197.8
c_{sat} ($J K^{-1} g^{-1}$)	1.912	1.948	1.985	2.023	2.062	2.101	2.142
C_{sat} ($J K^{-1} mol^{-1}$)	176.1	179.5	182.9	186.4	190.0	193.6	197.3
Temp. (K)	430	440	450	460	470	480	490
c_p ($J K^{-1} g^{-1}$)	2.191	2.239	2.291	2.349	2.412	2.483	2.561
C_p ($J K^{-1} mol^{-1}$)	201.9	206.3	211.1	216.4	222.3	228.8	236.0
c_{sat} ($J K^{-1} g^{-1}$)	2.185	2.231	2.280	2.334	2.394	2.460	2.533
C_{sat} ($J K^{-1} mol^{-1}$)	201.3	205.5	210.1	215.1	220.6	226.7	233.4
Temp. (K)	500						
c_p ($J K^{-1} g^{-1}$)	2.649						
C_p ($J K^{-1} mol^{-1}$)	244.1						
c_{sat} ($J K^{-1} g^{-1}$)	2.614						
C_{sat} ($J K^{-1} mol^{-1}$)	240.8						

TABLE 14.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	291	126	1.689	1.22–1	0.54	8.21–3	1 3
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
162.0–503.1	591.79	2.96623	3.04607–2	1.51030+1	3.32066	6.12322	1.97779+1	IV



Name: (Z)–Cycloheptene
Formula: C_7H_{12}

CAS–RN: 45510–00–7
Group No.: 14–012
Molar Mass: 96.17

TABLE 14.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89LEB/SMI	218.4–302.8	23	0.20	not specified		C_p	BSAO	76LEB/LIT

TABLE 14.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	22	0.984	3.69–2	0.20	1.26–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
218.5–302.8		1.49129+1	–4.01879–1	7.82994–1			III

TABLE 14.12.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.540	1.567	1.596	1.626	1.657	1.689	1.699
C_p (J K^{-1}mol^{-1})	148.2	150.7	153.5	156.3	159.3	162.4	163.4
Temp. (K)	280	290	298.15	300			
c_p (J K^{-1}g^{-1})	1.723	1.758	1.787	1.794			
C_p (J K^{-1}mol^{-1})	165.7	169.1	171.9	172.6			

TABLE 14.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	22	0.985	3.70–2	0.20	1.26–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
218.5–302.8	600.00	–4.95633	3.67604	9.13518	1.67063		III

Name: 1–Ethylcyclopentene
Formula: C_7H_{12}

CAS–RN: 2146–38–5
Group No.: 14–013
Molar Mass: 96.17

TABLE 14.13.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79FUC/PEA	298.15	1.958	1.50	99.	chrom	C_p	BSIO	80FUC

Name: 4–Methylcyclohexene
Formula: C_7H_{12}

CAS–RN: 591–47–9
Group No.: 14–014
Molar Mass: 96.17

TABLE 14.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88LEB/KUL	161.1–321.4	22	0.20	99.3	chrom	C_p	BSAO	76LEB/LIT

TABLE 14.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	1.794	7.25–2	0.36	4.54–4	–4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
161.1–321.4		1.61669+1	–8.75321–1	9.23000–1			III

TABLE 14.14.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J K^{-1}g^{-1}$)	1.481	1.500	1.520	1.542	1.566	1.591	1.617
C_p ($J K^{-1}mol^{-1}$)	142.4	144.2	146.2	148.3	150.6	153.0	155.6
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.646	1.676	1.707	1.740	1.775	1.786	1.811
C_p ($J K^{-1}mol^{-1}$)	158.3	161.2	164.2	167.4	170.7	171.8	174.2
Temp. (K)	290	298.15	300	310	320		
c_p ($J K^{-1}g^{-1}$)	1.849	1.881	1.889	1.930	1.973		
C_p ($J K^{-1}mol^{-1}$)	177.9	180.9	181.7	185.6	189.7		

TABLE 14.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	1.843	7.23–2	0.37	4.54–4	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
161.1–321.4	573.00	–3.04750	4.72273	9.40212	4.91626–1		III

Name: Ethynylbenzene
Formula: C_8H_6

CAS-RN: 536-74-3
Group No.: 14-015
Molar Mass: 102.14

TABLE 14.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31SMI/AND1	231.7–298.5	6	nosp	99.0	estim	C_p	DSIO	26AND/LYN
82LEB/BYK	228.0–330.0	4S	0.30	98.4	melpt	C_p	BSAO	76LEB/LIT

TABLE 14.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
31SMI/AND1	231.7–298.5	6	1.20#	0.934	2.28–1	1.12	–2.05–1	–6
82LEB/BYK	228.0–330.0	4	0.30	0.523	3.36–2	0.16	1.98–2	2

TABLE 14.15.3. Parameters of regression polynomial

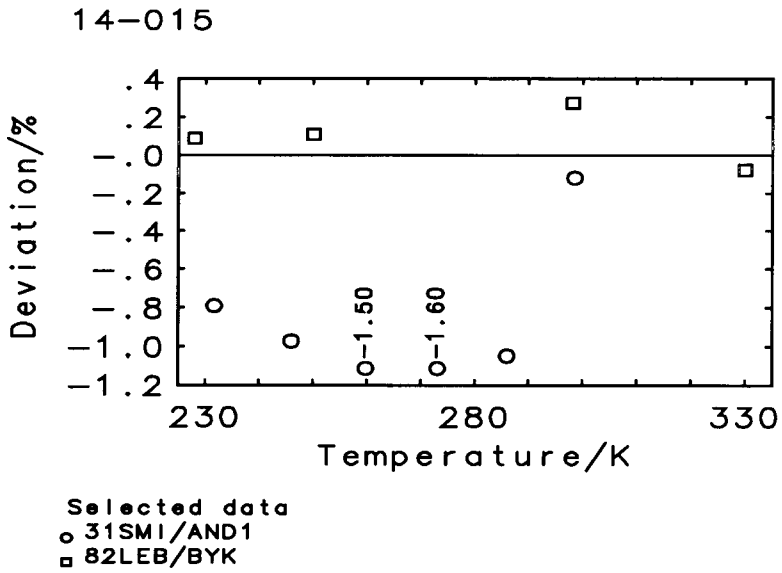
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.951	2.12–1	1.04	–1.15–1	–4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
228.0–330.0		1.89859+1	–1.61818	8.37050–1			IV

TABLE 14.15.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	1.603	1.622	1.642	1.664	1.687	1.694	1.711
C_p ($J K^{-1} mol^{-1}$)	163.7	165.7	167.7	169.9	172.3	173.0	174.8
Temp. (K)	290	298.15	300	310	320	330	
c_p ($J K^{-1} g^{-1}$)	1.737	1.759	1.764	1.792	1.822	1.853	
C_p ($J K^{-1} mol^{-1}$)	177.4	179.6	180.1	183.0	186.1	189.2	

TABLE 14.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	1.925	1.64–1	0.81	–2.97–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
228.0–330.0	643.70	–6.46565–2	6.56850	9.25609	1.59110–4		IV



Name: 1,3,5,7–Cyclooctatetraene
Formula: C_8H_8

CAS-RN: 629–20–9
Group No.: 14–016
Molar Mass: 104.15

TABLE 14.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49SCO/GRO	273.0–328.3	12	0.20	99.92	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 14.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.337	7.60–3	0.03	3.66–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–328.3		1.66604+1	7.53020–1	3.78797–1			II

TABLE 14.16.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.735	1.759	1.778	1.783	1.807	1.832	1.858
C_{sat} (J K^{-1}mol^{-1})	180.7	183.2	185.2	185.7	188.2	190.8	193.5

TABLE 14.16.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.344	7.76–3	0.03	3.97–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
273.0–328.3	639.00	–4.97768	9.43203–1	1.43124+1	6.56732		II

Name: Ethenylbenzene
Formula: C_8H_8

CAS-RN: 100–42–5
Group No.: 14–017
Molar Mass: 104.15

TABLE 14.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31SMI/AND1	246.0–298.5	5	nosp	99.0	estim	C_p	DSIO	26AND/LYN
46PIT/GUT	246.7–298.5	9	0.20	99.8	melpt	C_p	BSIO	28LAT/GRE
48TSC4	295.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC6	294.1	1	nosp	not specified		C_p	BSIO	48TSC1
50KUR	308.3–353.3	5	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 14.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
46PIT/GUT	246.7–298.5	9	0.20	1.541	6.36–2	0.31	4.14–4	3
				Rejected data				
31SMI/AND1	(3.24–1, 1.54, –3.17–1, –4)			48TSC4	(3.81–1, 1.78, –3.81–1, –1)			
48TSC6	(4.53–1, 2.12, –4.53–1, –1)							

TABLE 14.17.3. Parameters of regression polynomial

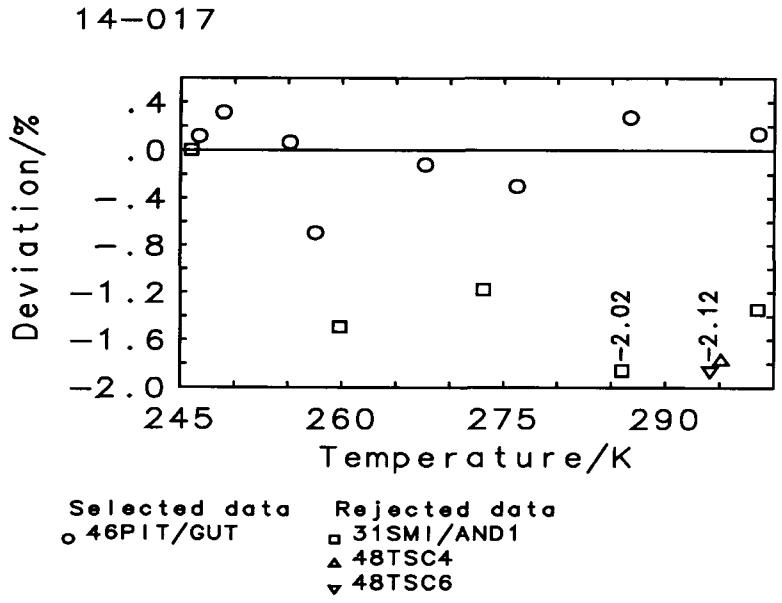
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	9	1.747	7.21–2	0.35	4.14–4	3
Temp. range K		A_1	A_2				Level of uncertainty
246.7–298.5		1.19343+1	3.34845				III

TABLE 14.17.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.621	1.648	1.674	1.683	1.701	1.728	1.750
C_p (J K^{-1}mol^{-1})	168.8	171.6	174.4	175.3	177.2	180.0	182.2
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.755						
C_p (J K^{-1}mol^{-1})	182.8						

TABLE 14.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	9	1.579	6.55–2	0.32	2.77–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
246.7–298.5	636.20	2.21355+1	1.73526+1	1.06718–2	7.05914		III



Name: 1,2–Dimethylbenzene
Formula: C_8H_{10}

CAS–RN: 95–47–6
Group No.: 14–018
Molar Mass: 106.17

TABLE 14.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24WIL/DAN		303.0–348.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
30HUF/PAR1		253.3–295.1	8	1.00	not specified		C_p	BSIO	25PAR
43PIT/SCO		251.6–301.9	9	0.20	99.88	melpt	C_p	BSIO	28LAT/GRE
47KUR		308.8–346.6	3	nosp	not specified		C_{avg}	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		C_p	BSIO	48TSC1
58SWI/ZIE2	N	347.3	1	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1
75RAS/GRI	N	303.2–463.1	10	1.00	not specified		C_p	BDAO	75RAS/GRI
77FOR/BEN		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
79FOR/BEN		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
93GAR/BAN		318.1–373.1	12	nosp	99.6	chrom	C_p	BDCT	91BAN/GAR

58SWI/ZIE2 average value in temperature range 333–373 K
75RAS/GRI data above 348 K measured at superambient pressures up to 0.51 MPa

TABLE 14.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
43PIT/SCO	251.6–301.9	9	0.20	1.263	5.64–2	0.25	7.83–3	2
75RAS/GRI	303.2–463.1	10	1.00	0.501	1.26–1	0.50	–2.22–2	–2
77FOR/BEN	298.1	1	0.50#	0.147	1.66–2	0.07	–1.66–2	–1
79FOR/BEN	298.1	1	0.30	0.123	8.32–3	0.04	–8.32–3	–1
91TAN/ADA	298.1	1	0.50#	0.162	1.83–2	0.08	–1.83–2	–1
93GAR/BAN	318.1–373.1	12	0.50#	0.418	4.91–2	0.21	–2.54–2	–4
				Rejected data				
24WIL/DAN	(7.05–1, 3.10, –7.02–1, –5)			30HUF/PAR1	(2.58–1, 1.19, –2.49–1, –8)			
47KUR	(2.09–1, 0.92, –1.37–1, –1)			48TSC3	(5.02–1, 2.29, –5.02–1, –1)			
48TSC6	(5.36–1, 2.45, –5.36–1, –1)			58SWI/ZIE2	(4.47–1, 1.80, 4.47–1, 1)			

TABLE 14.18.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	34	0.810	8.66–2	0.35	–1.47–2	–7
C_{sat}	53	34	0.809	8.65–2	0.35	–1.49–2	–7

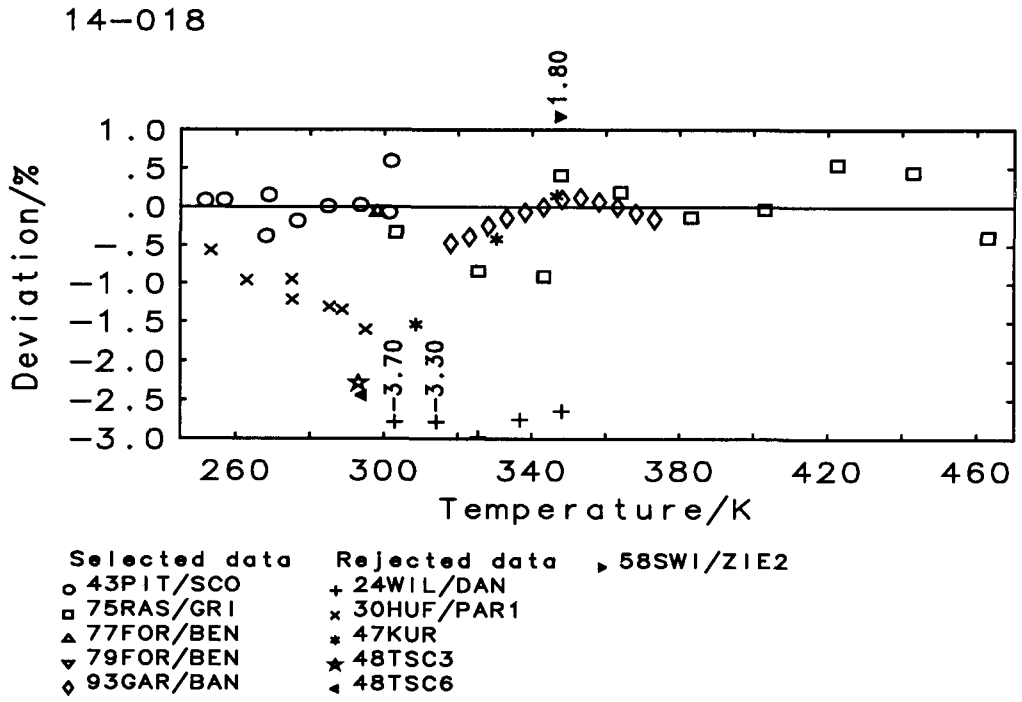
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
251.6–350.0	–4.59064	2.10061+1	–6.07675	7.00164–1	III
350.0–463.1	4.77123+1	–2.38250+1	6.73215	–5.19731–1	IV
251.6–350.0	–4.39299	2.08056+1	–6.00945	6.92696–1	III
350.0–463.1	4.94168+1	–2.53171+1	7.16845	–5.62343–1	IV

TABLE 14.18.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	1.636	1.664	1.692	1.701	1.719	1.746	1.768
C_p ($J K^{-1}mol^{-1}$)	173.6	176.7	179.7	180.6	182.5	185.4	187.7
c_{sat} ($J K^{-1}g^{-1}$)	1.636	1.664	1.692	1.701	1.719	1.746	1.768
C_{sat} ($J K^{-1}mol^{-1}$)	173.7	176.7	179.7	180.6	182.5	185.4	187.7
Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1}g^{-1}$)	1.773	1.800	1.828	1.857	1.888	1.920	1.953
C_p ($J K^{-1}mol^{-1}$)	188.3	191.1	194.1	197.2	200.4	203.8	207.4
c_{sat} ($J K^{-1}g^{-1}$)	1.773	1.800	1.828	1.857	1.888	1.920	1.953
C_{sat} ($J K^{-1}mol^{-1}$)	188.3	191.1	194.1	197.2	200.4	203.8	207.4
Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1}g^{-1}$)	1.989	2.026	2.064	2.104	2.144	2.185	2.226
C_p ($J K^{-1}mol^{-1}$)	211.2	215.1	219.2	223.4	227.6	231.9	236.3
c_{sat} ($J K^{-1}g^{-1}$)	1.989	2.026	2.064	2.103	2.143	2.183	2.223
C_{sat} ($J K^{-1}mol^{-1}$)	211.2	215.1	219.1	223.3	227.5	231.8	236.0
Temp. (K)	440	450	460				
c_p ($J K^{-1}g^{-1}$)	2.267	2.308	2.348				
C_p ($J K^{-1}mol^{-1}$)	240.7	245.0	249.3				
c_{sat} ($J K^{-1}g^{-1}$)	2.263	2.303	2.342				
C_{sat} ($J K^{-1}mol^{-1}$)	240.3	244.5	248.7				

TABLE 14.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	53	34	0.863	1.14–1	0.44	−7.53–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
251.6–463.1	630.30	−5.54618	8.70887−1	1.31753+1	8.83013		IV



Name: 1,3–Dimethylbenzene
Formula: C_8H_{10}

CAS–RN: 108–38–3
Group No.: 14–019
Molar Mass: 106.17

TABLE 14.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*86SCH		308.9–334.8	11S	nosp	not specified	C_{avg}	DSIO	*86SCH
24WIL/DAN		303.0–348.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
30HUF/PAR1	N	217.0–275.3	6	1.00	not specified	C_p	BSIO	25PAR
43PIT/SCO	N	231.4–318.2	11	0.20	97.66 melpt	C_p	BSIO	28LAT/GRE
47KUR		309.8–347.7	3	nosp	not specified	C_{avg}	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified	C_p	BSIO	48TSC1
58SWI/ZIE2	N	336.8	1	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
75RAS/GRI	N	302.9–462.5	9	1.00	not specified	C_p	BDAO	75RAS/GRI
75SAN	N	411.1–540.2	8S	1.00	not specified	C_p	FSIO	75SAN
77FOR/BEN		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
79FOR/BEN		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
93GAR/BAN		318.1–373.1	12	nosp	99.3 chrom	C_p	BDCT	91BAN/GAR

30HUF/PAR1 low sample purity
43PIT/SCO corrected for content of 1,4–Dimethylbenzene
58SWI/ZIE2 average value in temperature range 333–373 K
75RAS/GRI data above 384 K measured at superambient pressures up to 0.45 MPa
75SAN same data in 76SAN/MEL; C_p at saturation line extrapolated from high pressure measurement

TABLE 14.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
43PIT/SCO	231.4–318.2	11	0.20	1.597	6.72–2	0.32	1.24–2	3
75RAS/GRI	303.0–462.5	9	1.00	0.652	1.56–1	0.65	–5.34–2	–3
75SAN	411.1–540.2	8	1.00	0.723	2.28–1	0.72	8.12–2	4
93GAR/BAN	318.1–373.1	12	0.70#	0.847	1.41–1	0.59	–1.38–1	–12
				Rejected data				
*86SCH	(3.41–1, 1.44, 3.06–1, 11)			24WIL/DAN	(6.85–1, 3.07, –6.84–1, –5)			
30HUF/PAR1	(3.58–2, 0.17, 1.62–2, 0)			47KUR	(7.93–1, 3.24, 7.56–1, 3)			
48TSC3	(1.25–1, 0.58, –1.25–1, –1)			48TSC6	(1.58–1, 0.72, 1.58–1, 1)			
58SWI/ZIE2	(4.06–1, 1.70, 4.06–1, 1)			77FOR/BEN	(1.24–1, 0.57, –1.24–1, –1)			
79FOR/BEN	(1.16–1, 0.53, –1.16–1, –1)			91TAN/ADA	(1.41–1, 0.65, –1.41–1, –1)			

TABLE 14.19.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	71	40	1.130	1.62–1	0.62	–3.38–2	–8
C_{sat}	71	40	1.121	1.58–1	0.61	–3.40–2	–8

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
231.4–400.0	2.09114+1	–4.37338	2.00315	–1.40658–1	III
400.0–540.2	–1.66661+1	2.38098+1	–5.04264	4.46492–1	IV
231.4–400.0	2.10854+1	–4.56521	2.07307	–1.49080–1	III
400.0–540.2	–6.80272	1.63509+1	–3.15595	2.86672–1	IV

TABLE 14.19.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	1.546	1.567	1.590	1.614	1.640	1.648	1.667
C_p ($J\,K^{-1}mol^{-1}$)	164.1	166.4	168.8	171.4	174.1	175.0	177.0
c_{sat} ($J\,K^{-1}g^{-1}$)	1.546	1.567	1.590	1.614	1.640	1.648	1.667
C_{sat} ($J\,K^{-1}mol^{-1}$)	164.1	166.4	168.8	171.4	174.1	175.0	177.0

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	1.695	1.719	1.725	1.755	1.787	1.820	1.854
C_p ($J\,K^{-1}mol^{-1}$)	180.0	182.5	183.1	186.4	189.7	193.2	196.8
c_{sat} ($J\,K^{-1}g^{-1}$)	1.695	1.719	1.725	1.755	1.787	1.820	1.854
C_{sat} ($J\,K^{-1}mol^{-1}$)	180.0	182.5	183.1	186.4	189.7	193.2	196.8

Temp. (K)	350	360	370	380	390	400	410
c_p ($J\,K^{-1}g^{-1}$)	1.888	1.924	1.960	1.997	2.035	2.073	2.111
C_p ($J\,K^{-1}mol^{-1}$)	200.5	204.3	208.1	212.0	216.0	220.1	224.2
c_{sat} ($J\,K^{-1}g^{-1}$)	1.888	1.924	1.960	1.996	2.034	2.072	2.110
C_{sat} ($J\,K^{-1}mol^{-1}$)	200.5	204.2	208.1	212.0	215.9	219.9	224.0

Temp. (K)	420	430	440	450	460	470	480
c_p ($J\,K^{-1}g^{-1}$)	2.151	2.191	2.232	2.275	2.319	2.365	2.413
C_p ($J\,K^{-1}mol^{-1}$)	228.3	232.6	237.0	241.5	246.2	251.1	256.2
c_{sat} ($J\,K^{-1}g^{-1}$)	2.149	2.189	2.229	2.270	2.313	2.357	2.402
C_{sat} ($J\,K^{-1}mol^{-1}$)	228.1	232.3	236.6	241.0	245.6	250.2	255.0

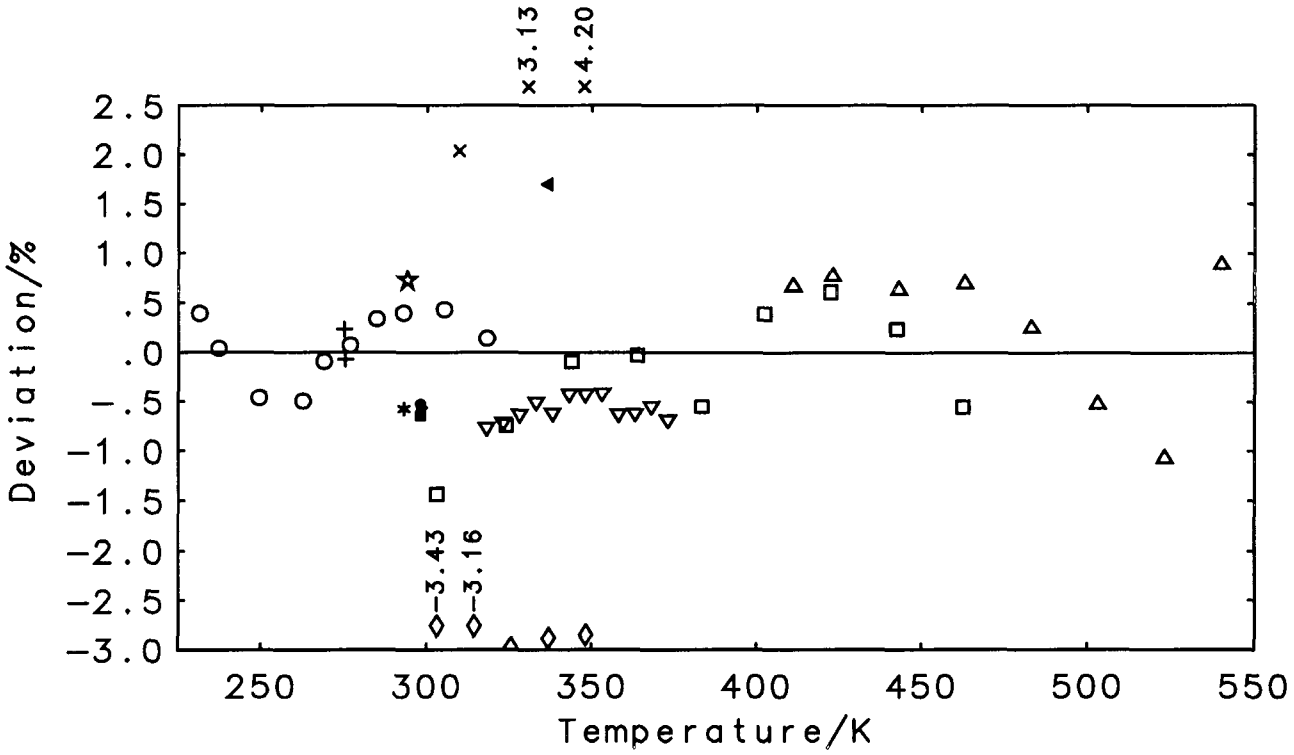
Temp. (K)	490	500	510	520	530	540
c_p ($J\,K^{-1}g^{-1}$)	2.464	2.516	2.571	2.629	2.690	2.754
C_p ($J\,K^{-1}mol^{-1}$)	261.6	267.1	273.0	279.1	285.6	292.4
c_{sat} ($J\,K^{-1}g^{-1}$)	2.449	2.497	2.547	2.600	2.654	2.710
C_{sat} ($J\,K^{-1}mol^{-1}$)	260.0	265.1	270.5	276.0	281.7	287.7

TABLE 14.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	71	40	1.244	1.63–1	0.58	1.63–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
231.4–540.2	617.05	8.32909–1	2.89196–3	1.59082+1	5.29671	1.20864+1	1.03672+1	IV

14–019



Selected data
- o 43PIT/SCO
- □ 75RAS/GRI
- △ 75SAN
- ▽ 93GAR/BAN

Rejected data
- ◇ 24WIL/DAN
- \+ 30HUF/PAR1
- × 47KUR
- ✱ 48TSC3
- ★ 48TSC6
- ◀ 58SWI/ZIE2
- ▶ 77FOR/BEN
- ● 79FOR/BEN
- ■ 91TAN/ADA

Name: 1,4–Dimethylbenzene
Formula: C_8H_{10}

CAS–RN: 106–42–3
Group No.: 14–020
Molar Mass: 106.17

TABLE 14.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH		312.2–335.7	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
24WIL/DAN		303.0–348.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
30HUF/PAR1		290.7–299.4	5	1.00	not specified		C_p	BSIO	25PAR
43PIT/SCO		292.0–354.6	10	0.20	99.98	melpt	C_p	BSIO	28LAT/GRE
47COR/GIN		293.1–573.2	15S	0.20	99.9	melpt	C_{sat}	DSTO	50GIN/DOU
47KUR		309.3–349.1	3	nosp	not specified		C_{avg}	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		C_p	BSIO	48TSC1
58SWI/ZIE2	N	336.6–347.0	2	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1
61ROU		298.0–315.9	20	nosp	not specified		C_p	BSAO	61ROU
71KHA/SUB	N	298.1–313.1	2	nosp	not specified		C_p	BSIO	64MOE/THO
75RAS/GRI	N	303.6–462.9	9	1.00	not specified		C_p	BDAO	75RAS/GRI
77FOR/BEN		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
77WIL/GRO		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
79FOR/BEN		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
79OTT/GOA		288.1–328.1	9S	0.30	99.9	melpt	C_p	FSIT	71PIC/LED
85COS/PAT7		298.2	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
88MES/FIN		295.4–373.4	11	0.10	99.996	melpt	C_{sat}	BSAO	47HUF
89PRA/RAJ		318.1–333.1	4	3.00	not specified		C_p	BDHT	89PRA/RAJ
91TAN/ADA		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
93GAR/BAN		318.1–373.1	12	nosp	99.7	chrom	C_p	BDCT	91BAN/GAR

58SWI/ZIE2 average values in temperature ranges 294–379 K and 295–399 K
71KHA/SUB reproducibility given as 0.3 %
75RAS/GRI data above 386 K measured at superambient pressures up to 0.49 MPa

TABLE 14.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47COR/GIN	293.1–573.2	15	0.20	1.405	7.36–2	0.28	–3.41–2	–5
75RAS/GRI	303.6–462.9	9	1.00	0.588	1.60–1	0.59	7.07–2	3
77FOR/BEN	298.1	1	0.50#	0.174	1.90–2	0.09	–1.90–2	–1
79FOR/BEN	298.1	1	0.30	0.027	1.77–3	0.01	–1.77–3	0
79OTT/GOA	288.1–328.1	9	0.30	0.852	5.71–2	0.26	–6.37–3	–3
88MES/FIN	295.4–373.4	11	0.20#	1.307	6.31–2	0.26	5.69–2	11
91TAN/ADA	298.1	1	0.50#	0.277	3.03–2	0.14	–3.03–2	–1
91WIL/JIM	298.1	1	0.50#	0.448	4.91–2	0.22	4.91–2	1
93GAR/BAN	318.1–373.1	12	0.70#	0.642	1.06–1	0.45	–1.02–1	–12
				Rejected data				
*86SCH	(2.96–1, 1.26, 2.82–1, 6)			24WIL/DAN	(7.04–1, 3.19, –6.96–1, –5)			
30HUF/PAR1	(2.06–1, 0.95, –1.99–1, –5)			43PIT/SCO	(4.51–1, 1.91, 1.97–1, 6)			
47KUR	(9.00–1, 3.68, 8.57–1, 3)			48TSC3	(3.12–1, 1.46, –3.12–1, –1)			
48TSC6	(2.99–1, 1.39, –2.99–1, –1)			58SWI/ZIE2	(3.52–1, 1.46, 3.52–1, 2)			
61ROU	(8.31–1, 3.60, 8.27–1, 20)			71KHA/SUB	(7.98–2, 0.36, –6.95–2, –2)			
77WIL/GRO	(4.83–2, 0.22, –4.83–2, –1)			85COS/PAT7	(2.02–1, 0.92, 2.02–1, 1)			
89PRA/RAJ	(3.48–1, 1.47, 3.24–1, 4)							

TABLE 14.20.3. Parameters of cubic spline polynomials

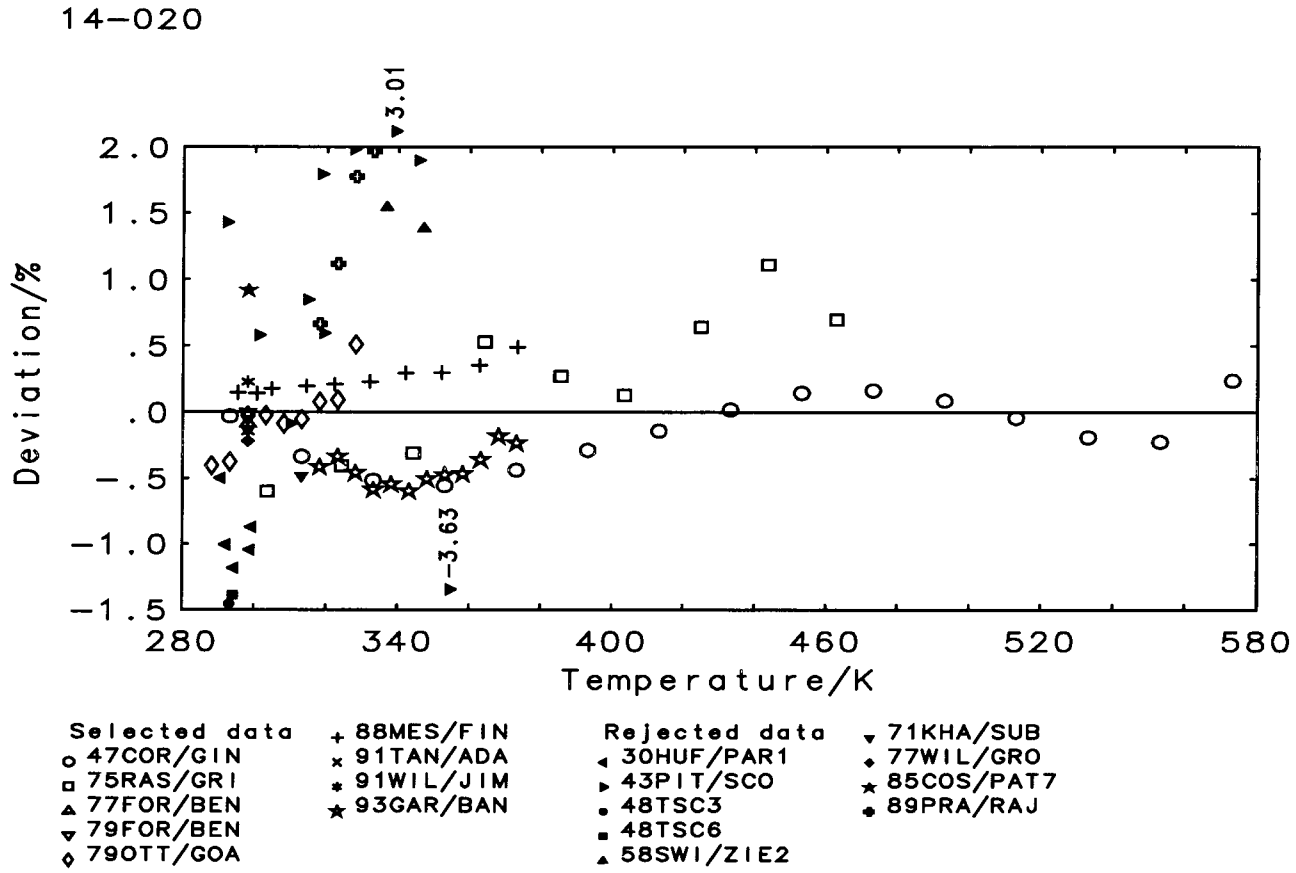
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	121	60	1.073	9.76–2	0.38	–8.94–3	–7
C_{sat}	121	60	1.020	9.40–2	0.38	–8.99–3	–7
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
288.1–420.0		1.78687+1	–2.57703	1.72250	–1.36338–1		II
420.0–573.2		–7.08471+1	6.07914+1	–1.33652+1	1.06110		IV
288.1–420.0		1.26505+1	1.77510	5.31803–1	–2.97523–2		II
420.0–573.2		–3.13461+1	3.32013+1	–6.95062	5.64090–1		IV

TABLE 14.20.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	1.688	1.714	1.720	1.752	1.785	1.819	1.853
C_p ($J\,K^{-1}mol^{-1}$)	179.2	182.0	182.6	186.0	189.5	193.1	196.7
c_{sat} ($J\,K^{-1}g^{-1}$)	1.687	1.714	1.720	1.753	1.786	1.819	1.853
C_{sat} ($J\,K^{-1}mol^{-1}$)	179.1	181.9	182.6	186.1	189.6	193.2	196.8
Temp. (K)	350	360	370	380	390	400	410
c_p ($J\,K^{-1}g^{-1}$)	1.888	1.923	1.959	1.994	2.031	2.067	2.104
C_p ($J\,K^{-1}mol^{-1}$)	200.4	204.2	207.9	211.8	215.6	219.5	223.3
c_{sat} ($J\,K^{-1}g^{-1}$)	1.888	1.922	1.957	1.993	2.028	2.064	2.100
C_{sat} ($J\,K^{-1}mol^{-1}$)	200.4	204.1	207.8	211.5	215.3	219.1	223.0
Temp. (K)	420	430	440	450	460	470	480
c_p ($J\,K^{-1}g^{-1}$)	2.140	2.177	2.214	2.252	2.292	2.334	2.378
C_p ($J\,K^{-1}mol^{-1}$)	227.2	231.1	235.1	239.1	243.4	247.8	252.5
c_{sat} ($J\,K^{-1}g^{-1}$)	2.137	2.173	2.211	2.249	2.288	2.328	2.370
C_{sat} ($J\,K^{-1}mol^{-1}$)	226.8	230.7	234.7	238.7	242.9	247.2	251.6
Temp. (K)	490	500	510	520	530	540	550
c_p ($J\,K^{-1}g^{-1}$)	2.425	2.476	2.531	2.590	2.654	2.724	2.800
C_p ($J\,K^{-1}mol^{-1}$)	257.5	262.9	268.7	275.0	281.8	289.2	297.2
c_{sat} ($J\,K^{-1}g^{-1}$)	2.414	2.460	2.508	2.559	2.612	2.669	2.730
C_{sat} ($J\,K^{-1}mol^{-1}$)	256.3	261.1	266.2	271.6	277.4	283.4	289.8
Temp. (K)	560	570					
c_p ($J\,K^{-1}g^{-1}$)	2.882	2.971					
C_p ($J\,K^{-1}mol^{-1}$)	306.0	315.4					
c_{sat} ($J\,K^{-1}g^{-1}$)	2.794	2.862					
C_{sat} ($J\,K^{-1}mol^{-1}$)	296.6	303.8					

TABLE 14.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	121	60	1.165	8.81–2	0.35	–1.65–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
288.1–573.2	616.20	–3.18089	1.32290–1	1.02433+1	1.91210+1		IV



Name: Ethylbenzene
Formula: C_8H_{10}

CAS–RN: 100–41–4
Group No.: 14–021
Molar Mass: 106.17

TABLE 14.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON		304.8–362.1	8S	nosp	not specified	C_{avg}	DSIO	*81VON
*86SCH		309.0–335.7	11S	nosp	not specified	C_{avg}	DSIO	*86SCH
24WIL/DAN		303.0–343.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
30HUF/PAR1		185.0–304.9	16	1.00	not specified	C_p	BSIO	25PAR
31BLA/LEI		286.1–368.1	25	3.00	not specified	C_{sat}	BSIO	31BLA/LEI
31SMI/AND1		184.4–298.5	9	nosp	99.9 estim	C_p	DSIO	26AND/LYN
34KOL/UDO2	N	302.7	1	nosp	not specified	C_p	BSIT	34KOL/UDO2
44GUT/SPI		181.5–305.4	16	0.20	99.93 melpt	C_p	BSAO	43RUE/HUF
45SCO/BRI		178.2–300.0	27S	0.10	99.993 melpt	C_{sat}	BSAO	33SOU/BRI
47KUR		308.8–372.8	4	nosp	not specified	C_{avg}	DSIO	47KUR
48TSC1		295.1	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC5		295.1	1	nosp	not specified	C_p	BSIO	48TSC1
76FOR/BEN2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
77FOR/BEN		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
79AND/GRI	N	293.3–393.0	10	0.50	not specified	C_{sat}	BSAO	67RAS/GAN
79FOR/BEN		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
83GRO/FAR1		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
91TAN/ADA		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
91WIL/JIM		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
93GAR/BAN		318.1–373.1	12	nosp	99.5 chrom	C_p	BDCT	91BAN/GAR

34KOL/UDO2 same datum in 34KOL/UDO1
79AND/GRI error 0.5 % below 373 K and 0.8 % at 433 K

TABLE 14.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
44GUT/SPI	181.5–305.4	16	0.20#	0.322	1.36–2	0.06	–9.97–3	–11
45SCO/BRI	178.1–300.0	27	0.10	0.319	6.89–3	0.03	2.40–3	9
76FOR/BEN2	298.1	1	0.30	0.246	1.65–2	0.07	–1.65–2	–1
77FOR/BEN	298.1	1	0.50#	0.386	4.31–2	0.19	–4.31–2	–1
79AND/GRI	293.3–393.0	10	0.50	0.525	6.53–2	0.26	5.44–3	–2
83GRO/FAR1	298.1	1	0.50#	0.169	1.89–2	0.08	–1.89–2	–1
91WIL/JIM	298.1	1	0.50#	0.137	1.53–2	0.07	–1.53–2	–1
93GAR/BAN	318.1–373.1	12	0.70#	0.801	1.32–1	0.56	–8.76–2	–7
				Rejected data				
*81VON	(3.15–1, 1.30, –3.03–3, 2)			*86SCH	(3.40–1, 1.42, 3.22–1, 11)			
24WIL/DAN	(6.17–1, 2.73, –6.12–1, –5)			30HUF/PAR1	(3.01–1, 1.40, –2.58–1, –16)			
31BLA/LEI	(9.06–1, 3.56, 4.56–1, 15)			31SMI/AND1	(4.53–1, 2.35, –4.27–1, –9)			
34KOL/UDO2	(1.04, 4.84, –1.04, –1)			47KUR	(8.43–1, 3.23, 7.21–1, 4)			
48TSC1	(3.75–2, 0.17, 3.75–2, 1)			48TSC5	(1.44–1, 0.64, 1.44–1, 1)			
79FOR/BEN	(4.15–2, 0.19, –4.15–2, –1)			91TAN/ADA	(3.82–2, 0.17, –3.82–2, –1)			

TABLE 14.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	152	69	0.482 6.	32–2	0.27	–1.72–2	–15
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
178.1–393.0		2.48043+1	–9.01410	3.87757	–3.78713–1		IV

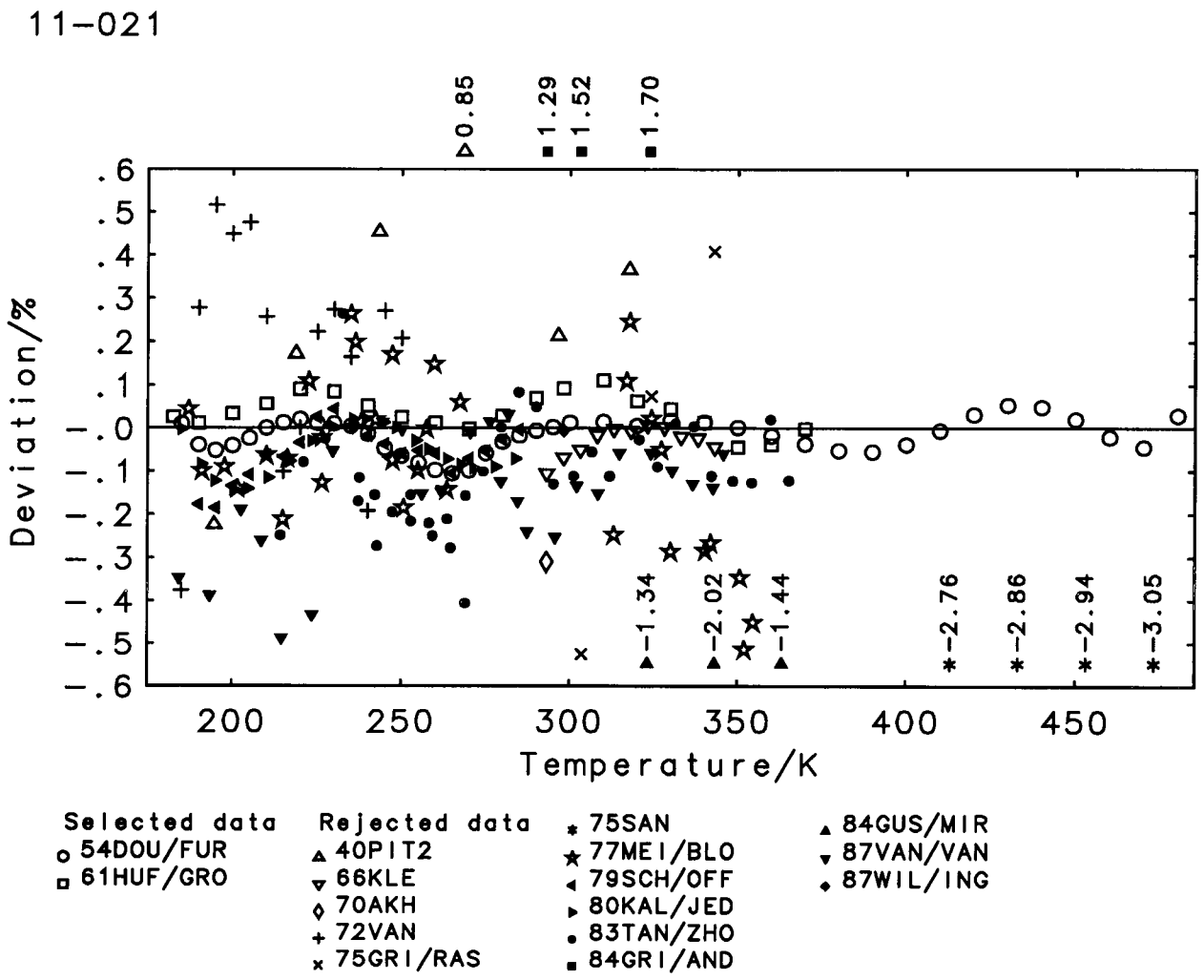
TABLE 14.21.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c ($J K^{-1} g^{-1}$)	1.483	1.494	1.508	1.525	1.543	1.564	1.587
C ($J K^{-1} mol^{-1}$)	157.4	158.6	160.1	161.9	163.9	166.1	168.5
Temp. (K)	250	260	270	273.15	280	290	298.15
c ($J K^{-1} g^{-1}$)	1.612	1.639	1.667	1.676	1.696	1.726	1.751
C ($J K^{-1} mol^{-1}$)	171.2	174.0	176.9	177.9	180.0	183.2	185.9
Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	1.757	1.789	1.821	1.854	1.887	1.920	1.953
C ($J K^{-1} mol^{-1}$)	186.5	189.9	193.4	196.8	200.3	203.9	207.3
Temp. (K)	370	380	390				
c ($J K^{-1} g^{-1}$)	1.986	2.018	2.049				
C ($J K^{-1} mol^{-1}$)	210.8	214.2	217.5				

TABLE 14.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	152	69	0.718	7.88–2	0.33	–1.20–2	–7

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
178.1–393.0	617.24	3.16141+2	3.04404+1	–1.23068+1	2.89465+2	8.96899+1	2.09550+2	IV



Name: Bicyclo[2.2.2]oct–2–ene
Formula: C_8H_{12}

CAS–RN: 931–64–6
Group No.: 14–022
Molar Mass: 108.18

TABLE 14.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70WON/WES	392.5–408.3	7	nosp	99.82	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 14.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	1.021	8.31–2	0.31	3.67–4	1
Temp. range K		A_1	A_2				Level of uncertainty
392.5–408.3		8.10580–1	6.60379				III

TABLE 14.22.4. Recommended values of heat capacities

Temp. (K)	390	400	410
c_{sat} (J K^{-1}g^{-1})	2.042	2.092	2.143
C_{sat} (J K^{-1}mol^{-1})	220.9	226.4	231.9

Name: 1,5–Cyclooctadiene (unspecified stereoisomer)
Formula: C_8H_{12}

CAS–RN: 111–78–4
Group No.: 14–023
Molar Mass: 108.18

TABLE 14.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75LEB/TSV	N	207.5–320.0	27	0.20	99.53	melpt	C_p	BSAO	66NIK/LEB

75LEB/TSV smoothed values in 75LEB/LEB

TABLE 14.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	27	0.208	9.08–3	0.04	6.15–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
207.4–320.0		2.46266+1	–9.17333	4.28360	–4.30880–1		III

TABLE 14.23.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.557	1.582	1.610	1.639	1.670	1.703	1.737
C_p (J K^{-1}mol^{-1})	168.5	171.2	174.2	177.3	180.7	184.2	188.0
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.748	1.773	1.809	1.840	1.846	1.884	1.923
C_p (J K^{-1}mol^{-1})	189.1	191.8	195.7	199.0	199.8	203.9	208.0

TABLE 14.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	27	0.500	2.22–2	0.10	3.72–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
207.4–320.0	647.00	–5.54551	6.01692	8.74044	1.27776	III

Name: Cyclooctene (unspecified stereoisomer)
Formula: C_8H_{14}

CAS–RN: 931–88–4
Group No.: 14–024
Molar Mass: 110.20

TABLE 14.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78LEB/LEB	N	260.9–328.2	31	0.20	99.978	melpt	C_p	BSAO	76LEB/LIT

78LEB/LEB probably *cis*–isomer (according to n.m.t. and diferent stability of both stereoisomers)

TABLE 14.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	30	1.442	7.22–2	0.29	3.84–4	4

Temp. range K	A_1	A_2	Level of uncertainty
262.2–328.2	8.50675	5.52350	III

TABLE 14.24.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.725	1.767	1.780	1.809	1.850	1.884	1.892
C_p (J K^{-1}mol^{-1})	190.1	194.7	196.2	199.3	203.9	207.7	208.5

Temp. (K)	310	320	330
c_p (J K^{-1}g^{-1})	1.934	1.975	2.017
C_p (J K^{-1}mol^{-1})	213.1	217.7	222.3

TABLE 14.24.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	30	1.467	7.36–2	0.29	3.86–4	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
262.2–328.2	617.00	1.24672	1.06690–2	8.18025	3.64211+1	III

Name: 1*H*–Indene
Formula: C_9H_8

CAS-RN: 95–13–6
Group No.: 14–025
Molar Mass: 116.16

TABLE 14.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61STU/SIN	N	280.0–300.0	3S	0.25	99.7	melpt	C_p	BSAO	58HIL/KRA
65ZIE	N	315.7–375.1	3	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1

61STU/SIN same data in 59STU/SIN
65ZIE average values in temperature ranges 296–454 K, 294–382 K and 294–338 K

TABLE 14.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61STU/SIN	280.0–300.0	3	0.25	0.141	7.71–3	0.04	1.77–3	0
65ZIE	315.7–375.1	3	1.50#	0.877	3.24–1	1.32	–5.34–2	–1

TABLE 14.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.770	2.80–1	1.14	–2.58–2	–1

Temp. range K	A_1	A_2	Level of uncertainty
280.0–375.1	1.03749+1	4.06333	V

TABLE 14.25.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.56	1.59	1.61	1.62	1.64	1.67	1.70
C_p (J K^{-1}mol^{-1})	181	184	187	188	191	194	198
Temp. (K)	340	350	360	370			
c_p (J K^{-1}g^{-1})	1.73	1.76	1.79	1.82			
C_p (J K^{-1}mol^{-1})	201	205	208	211			

Name: 2,3–Dihydroindene
Formula: C_9H_{10}

CAS–RN: 496–11–7
Group No.: 14–026
Molar Mass: 118.18

TABLE 14.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61STU/SIN	N	240.0–320.0	6S	0.25	99.89	melpt	C_p	BSAO	58HIL/KRA

61STU/SIN same data in 59STU/SIN

TABLE 14.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.533	3.02–2	0.13	4.58–5	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
240.0–320.0		2.13733+1	–3.96813	1.49978			II

TABLE 14.26.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	1.441	1.465	1.491	1.519	1.528	1.549	1.582
C_p ($J K^{-1} mol^{-1}$)	170.4	173.2	176.2	179.5	180.6	183.1	186.9
Temp. (K)	298.15	300	310	320			
c_p ($J K^{-1} g^{-1}$)	1.609	1.616	1.652	1.691			
C_p ($J K^{-1} mol^{-1}$)	190.2	191.0	195.3	199.8			

TABLE 14.26.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.450	2.56–2	0.11	2.80–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
240.0–320.0	684.90	1.83258+1	1.98319+1	–3.62235	4.23351		II

Name: (1–Methylethenyl)benzene
Formula: C_9H_{10}

CAS–RN: 98–83–9
Group No.: 14–027
Molar Mass: 118.18

TABLE 14.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67LEB/RAB1	N	250.8–300.0	6S	0.50	99.5	melpt	C_p	BSAO	66NIK/LEB

67LEB/RAB1 same data in 71LEB/RAB2

TABLE 14.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.626	7.45–2	0.31	3.44–4	0
Temp. range K		A_1	A_2				Level of uncertainty
250.8–300.0		1.23867+1	3.94111				IV

TABLE 14.27.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	1.592	1.620	1.629	1.648	1.676	1.698	1.703
C_p ($J\,K^{-1}mol^{-1}$)	188.2	191.5	192.5	194.7	198.0	200.7	201.3

Name: (1–Methylethyl)benzene
Formula: C_9H_{12}

CAS–RN: 98–82–8
Group No.: 14–028
Molar Mass: 120.19

TABLE 14.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
34KOL/UDO2	N	302.0	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
47KUR		308.8–359.6	4	nosp	not specified		C_{avg}	DSIO	47KUR
52SCH/SAG		299.8–366.5	13S	1.00	99.8	estim	C_p	BSAO	39SAG/EVA
73KIS/SUG		179.9–313.1	45	nosp	99.93	melpt	C_{sat}	BSAO	65SUG/SEK
79AND/GRI	N	296.0–412.8	7	0.50	not specified		C_{sat}	BSAO	67RAS/GAN

34KOL/UDO2 same datum in 34KOL/UDO1
79AND/GRI error 0.5 % below 373 K and 0.8 % at 433 K

TABLE 14.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KIS/SUG	179.9–313.1	45	0.20#	0.362	1.78–2	0.07	1.65–3	0
79AND/GRI	296.0–412.8	7	0.50	0.728	1.03–1	0.36	–6.45–2	–3
				Rejected data				
34KOL/UDO2	(2.14, 8.96, –2.14, –1)		47KUR	(1.51–1, 0.55, –7.02–2, –2)				
52SCH/SAG	(4.93–1, 1.91, –3.84–1, –9)							

TABLE 14.28.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	70	52	0.452	4.35–2	0.16	–7.25–3	–3

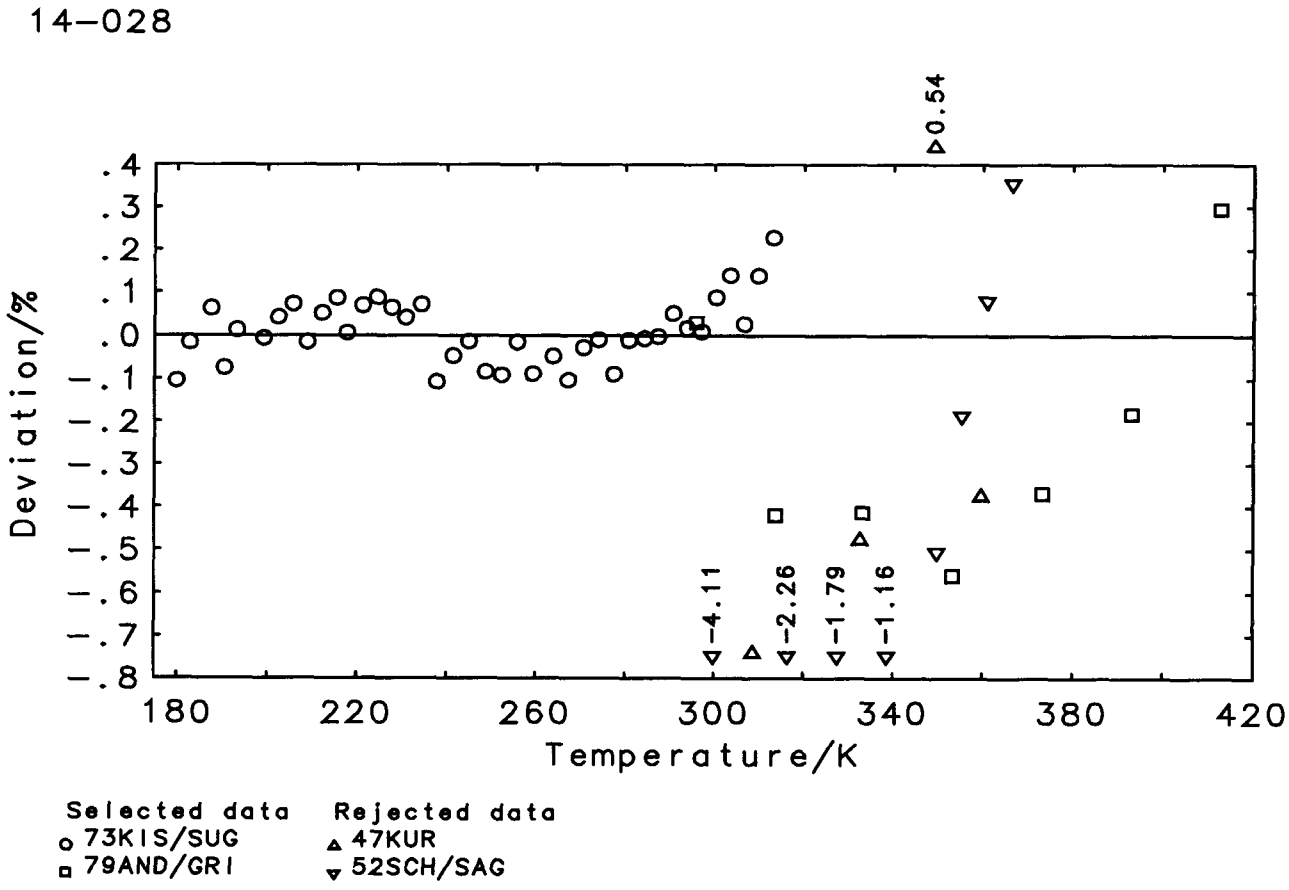
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
179.9–300.0	2.77820+1	–1.01809+1	4.62002	–4.75860–1	II
300.0–412.8	1.83532+1	–7.52100–1	1.47708	–1.26645–1	IV

TABLE 14.28.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} ($J K^{-1} g^{-1}$)	1.498	1.512	1.528	1.547	1.569	1.592	1.617
C_{sat} ($J K^{-1} mol^{-1}$)	180.0	181.7	183.7	186.0	188.6	191.4	194.4
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J K^{-1} g^{-1}$)	1.644	1.673	1.702	1.712	1.733	1.764	1.791
C_{sat} ($J K^{-1} mol^{-1}$)	197.6	201.0	204.6	205.7	208.3	212.1	215.2
Temp. (K)	300	310	320	330	340	350	360
c_{sat} ($J K^{-1} g^{-1}$)	1.797	1.829	1.862	1.896	1.930	1.964	1.998
C_{sat} ($J K^{-1} mol^{-1}$)	215.9	219.9	223.8	227.9	231.9	236.0	240.1
Temp. (K)	370	380	390	400	410		
c_{sat} ($J K^{-1} g^{-1}$)	2.032	2.067	2.101	2.136	2.170		
C_{sat} ($J K^{-1} mol^{-1}$)	244.3	248.4	252.5	256.7	260.8		

TABLE 14.28.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	70	52	0.578	7.33–2	0.25	–9.51–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
179.9–412.8	631.10	2.53596+2	2.31237+1	–2.73796	2.30950+2	9.16085+1	1.65041+2	III



Name: Propylbenzene
Formula: C_9H_{12}

CAS-RN: 103-65-1
Group No.: 14-029
Molar Mass: 120.19

TABLE 14.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*86SCH	308.6–346.9	9S	nosp	not specified	C_{avg}	DSIO	*86SCH
48TSC1	295.1	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC5	294.1	1	nosp	not specified	C_p	BSIO	48TSC1
65MES/TOD2	180.9–370.5	23	0.20	99.97 melpt	C_{sat}	BSAO	47HUF
83GRO/FAR2	298.1	1	nosp	99.0 estim	C_p	FSIT	71PIC/LED

TABLE 14.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65MES/TOD2	180.9–370.5	23	0.20#	0.116	6.07–3	0.02	1.82–6	4
				Rejected data				
*86SCH	(4.51–1, 1.58, 3.95–1, 9)			48TSC1	(3.45–2, 0.13, –3.45–2, –1)			
48TSC5	(4.90–2, 0.19, –4.90–2, –1)			83GRO/FAR2	(4.40–2, 0.17, –4.40–2, –1)			

TABLE 14.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	35	23	0.127	6.68–3	0.03	1.82–6	4
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
180.9–370.5	2.93134+1	–1.08270+1	4.52644	–4.32074–1			II

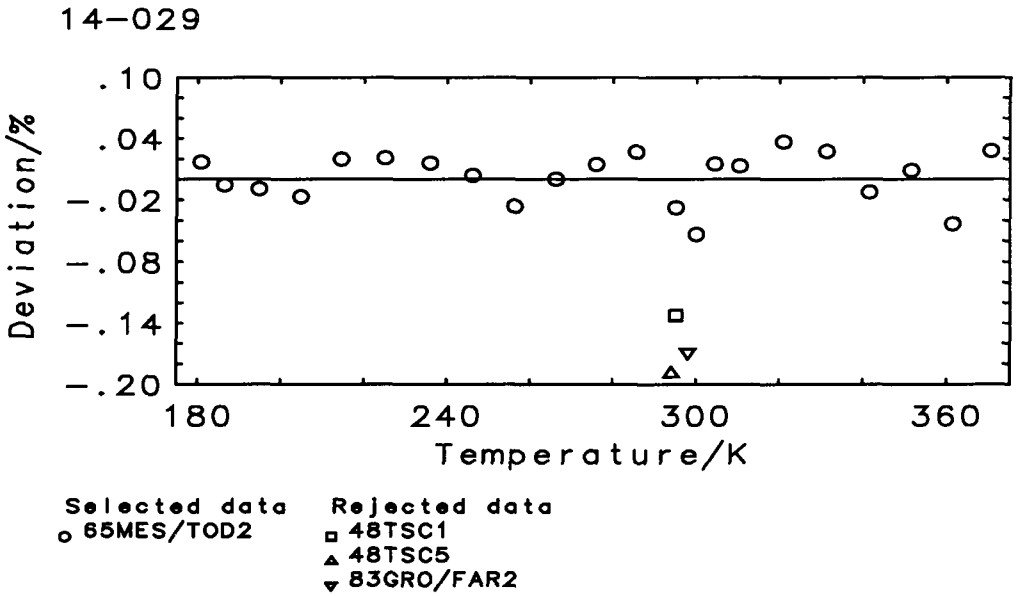
TABLE 14.29.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.520	1.530	1.543	1.559	1.577	1.598	1.621
C_{sat} (J K^{-1}mol^{-1})	182.7	183.9	185.5	187.4	189.6	192.1	194.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.645	1.672	1.700	1.709	1.729	1.760	1.786
C_{sat} (J K^{-1}mol^{-1})	197.8	200.9	204.3	205.4	207.9	211.6	214.7
Temp. (K)	300	310	320	330	340	350	360
c_{sat} (J K^{-1}g^{-1})	1.792	1.825	1.858	1.892	1.926	1.961	1.995
C_{sat} (J K^{-1}mol^{-1})	215.4	219.3	223.3	227.4	231.5	235.7	239.8
Temp. (K)	370						
c_{sat} (J K^{-1}g^{-1})	2.029						
C_{sat} (J K^{-1}mol^{-1})	243.9						

TABLE 14.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	35	23	0.343	1.72–2	0.07	2.86–5	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
180.9–370.5	638.30	4.95451+2	4.98904+1	–2.88255+1	4.52545+2	1.35495+2	3.13175+2	II



Name: 1,2,3–Trimethylbenzene
Formula: C_9H_{12}

CAS–RN: 526–73–8
Group No.: 14–030
Molar Mass: 120.19

TABLE 14.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55TAY/JOH	250.0–301.0	27	0.30	99.99	melpt	C_p	BSIO	55TAY/JOH

TABLE 14.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	27	1.111	8.32–2	0.33	5.24–4	8

Temp. range K	A_1	A_2	Level of uncertainty
250.0–301.0	1.44581+1	3.85259	III

TABLE 14.30.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	1.666	1.693	1.720	1.728	1.746	1.773	1.795
C_p ($J K^{-1}mol^{-1}$)	200.3	203.5	206.7	207.7	209.9	213.1	215.7
Temp. (K)	300						
c_p ($J K^{-1}g^{-1}$)	1.800						
C_p ($J K^{-1}mol^{-1}$)	216.3						

TABLE 14.30.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	27	27	1.086	8.13-2	0.33	4.72-4	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
250.0–301.0	664.47	5.99939	1.21025+1	7.27473	7.43496-1		III

Name: 1,2,4-Trimethylbenzene
Formula: C_9H_{12}

CAS-RN: 95-63-6
Group No.: 14-031
Molar Mass: 120.19

TABLE 14.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH		309.3–346.1	8S	nosp	not specified		C_{avg}	DSIO	*86SCH
31HUF/PAR		239.5–297.3	7	1.00	not specified		C_p	BSIO	25PAR
47KUR	N	308.6–365.3	5	nosp	not specified		C_{avg}	DSIO	47KUR
48TSC3		293.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified		C_p	BSIO	48TSC1
55HEL/HEI		294.3–377.6	16S	nosp	99.4	melpt	C_p	BSAO	39SAG/EVA
57PUT/KIL		230.2–301.0	39	0.30	99.7	melpt	C_p	BSIO	55TAY/JOH
79AND/GRI	N	293.1–429.9	19	0.50	not specified		C_{sat}	BSAO	67RAS/GAN
87WIL/ING		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

47KUR estimated error about 5%
79AND/GRI error 0.5 % below 373 K and 0.8 % at 433 K

TABLE 14.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
57PUT/KIL	230.2–301.0	39	0.30	0.343	2.60-2	0.10	5.91-3	4
79AND/GRI	293.1–429.9	19	0.50	0.713	9.96-2	0.36	-3.27-2	-7
				Rejected data				
*86SCH	(3.47-1, 1.25, 1.70-1, 0)			31HUF/PAR	(1.31-1, 0.53, -1.19-1, -7)			
47KUR	(4.43-1, 1.54, 3.55-1, 5)			48TSC3	(4.90-1, 1.95, -4.90-1, -1)			
48TSC6	(6.51-1, 2.61, -6.51-1, -1)			55HEL/HEI	(3.82-1, 1.47, -2.96-1, -10)			
87WIL/ING	(1.61-1, 0.63, -1.61-1, -1)							

TABLE 14.31.3. Parameters of cubic spline polynomials

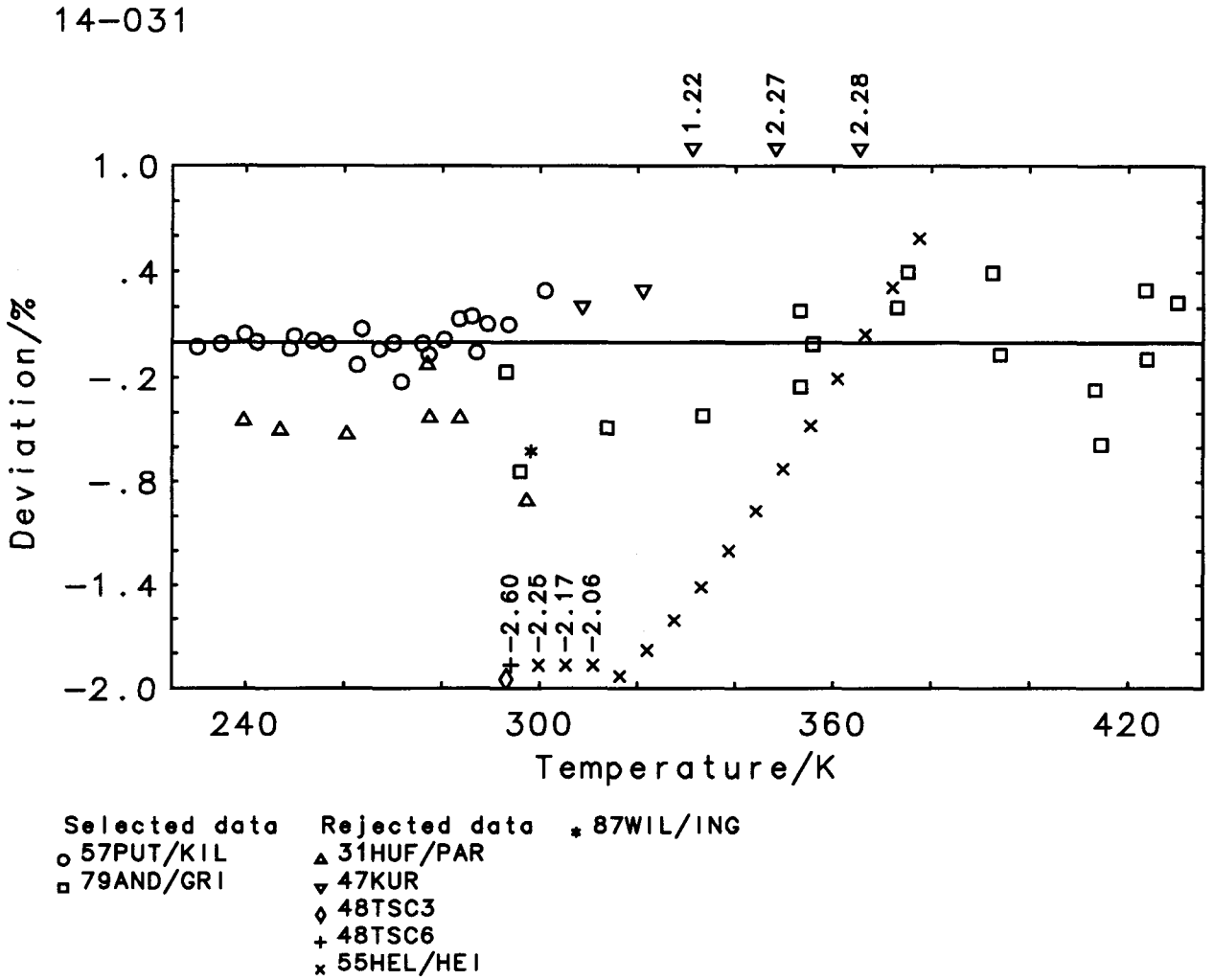
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	97	58	0.518	6.36–2	0.23	–6.74–3	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
230.2–330.0		2.61593+1	–7.85653	3.79254	–4.02072–1		II
330.0–429.9		–2.66111+1	4.01166+1	–1.07448+1	1.06634		III

TABLE 14.31.4. *Recommended values of heat capacities*

Temp. (K)	230	240	250	260	270	273.15	280
c ($J K^{-1} g^{-1}$)	1.609	1.632	1.656	1.681	1.707	1.716	1.734
C ($J K^{-1} mol^{-1}$)	193.4	196.1	199.0	202.1	205.2	206.2	208.4
Temp. (K)	290	298.15	300	310	320	330	340
c ($J K^{-1} g^{-1}$)	1.762	1.784	1.789	1.817	1.846	1.874	1.901
C ($J K^{-1} mol^{-1}$)	211.7	214.4	215.1	218.4	221.8	225.2	228.5
Temp. (K)	350	360	370	380	390	400	410
c ($J K^{-1} g^{-1}$)	1.930	1.958	1.988	2.019	2.052	2.088	2.127
C ($J K^{-1} mol^{-1}$)	231.9	235.4	238.9	242.7	246.7	251.0	255.6
Temp. (K)	420	430					
c ($J K^{-1} g^{-1}$)	2.168	2.2137					
C ($J K^{-1} mol^{-1}$)	260.6	266.07					

TABLE 14.31.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	97	58	0.580	6.65–2	0.24	–4.39–3	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
230.2–429.9	649.17	–6.20509	8.79443–1	1.52893+1	1.09453+1		III



Name: 1,3,5–Trimethylbenzene
Formula: C_9H_{12}

CAS–RN: 108–67–8
Group No.: 14–032
Molar Mass: 120.19

TABLE 14.32.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		303.9–348.8	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*86SCH		320.5–349.4	8S	nosp	not specified		C_{avg}	DSIO	*86SCH
47KUR		309.9–359.3	5	nosp	not specified		C_{avg}	DSIO	47KUR
55HEL/HEI		294.3–377.6	16S	nosp	99.78	melpt	C_p	BSAO	39SAG/EVA
55TAY/KIL		230.0–304.5	20	0.30	99.95	melpt	C_p	BSIO	55TAY/JOH
65ZIE	N	315.6–366.3	3	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1
68REC1	N	298.0–313.0	eqn	nosp	not specified		C_p	BSAO	68REC1
77FOR/BEN		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
79AND/GRI	N	295.0–423.6	8	0.50	not specified		C_{sat}	BSAO	67RAS/GAN
79WIL/FAR		298.1	1	0.30	99.0	estim	C_p	FSIT	71PIC/LED

65ZIE average values in temperature ranges 295–438 K and 294–338 K
68REC1 same data in 68REC2
79AND/GRI error 0.5 % below 373 K and 0.8 % at 433 K

TABLE 14.32.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
55TAY/KIL	230.0–304.5	20	0.30	0.644	4.72–2	0.19	1.52–2	1
77FOR/BEN	298.1	1	0.30	1.104	8.27–2	0.33	–8.27–2	–1
79AND/GRI	295.0–423.6	8	0.50	0.792	1.05–1	0.40	–4.44–2	0
79WIL/FAR	298.1	1	0.30	1.152	8.63–2	0.35	–8.63–2	–1
				Rejected data				
*81VON	(7.03–1, 2.60, 6.97–1, 4)			*86SCH	(8.94–1, 3.22, 8.73–1, 8)			
47KUR	(8.63–1, 3.11, 8.41–1, 5)			55HEL/HEI	(5.70–1, 2.22, –9.70–2, –2)			
65ZIE	(1.13–1, 0.42, –4.92–2, 1)			68REC1	(1.95–1, 0.78, –1.94–1, –5)			

TABLE 14.32.3. Parameters of regression polynomial

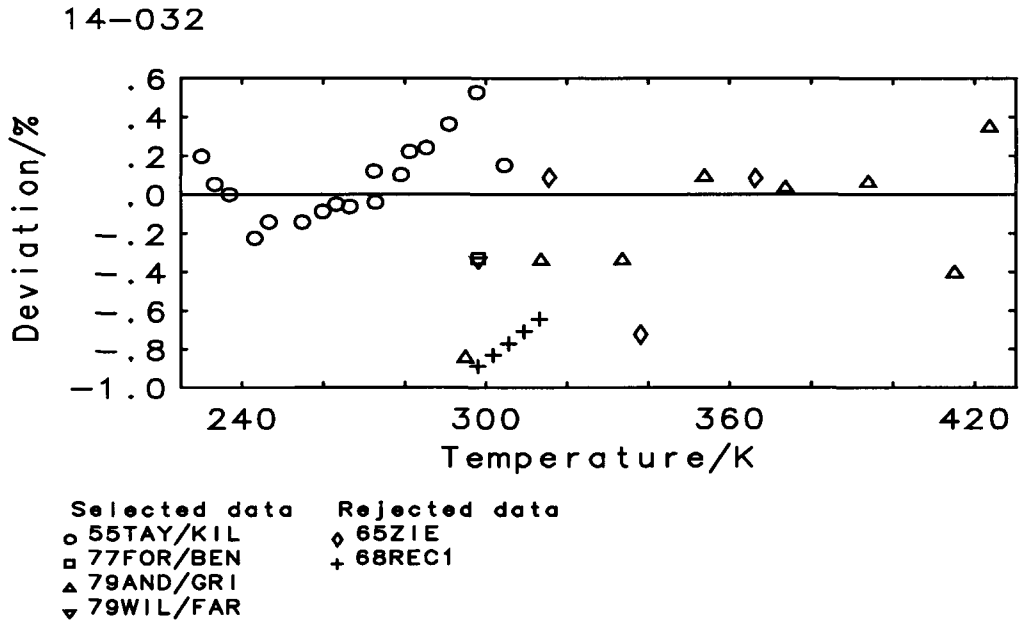
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	71	30	0.781	7.53–2	0.29	–7.34–3	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
230.0–423.6		7.97146	9.81903	–2.22329	2.85949–1		III

TABLE 14.32.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c ($J K^{-1} g^{-1}$)	1.541	1.569	1.597	1.625	1.654	1.662	1.682
C ($J K^{-1} mol^{-1}$)	185.2	188.6	192.0	195.4	198.7	199.8	202.1
Temp. (K)	290	298.15	300	310	320	330	340
c ($J K^{-1} g^{-1}$)	1.710	1.734	1.739	1.768	1.798	1.829	1.860
C ($J K^{-1} mol^{-1}$)	205.6	208.4	209.0	212.5	216.1	219.8	223.6
Temp. (K)	350	360	370	380	390	400	410
c ($J K^{-1} g^{-1}$)	1.893	1.926	1.961	1.997	2.035	2.074	2.114
C ($J K^{-1} mol^{-1}$)	227.5	231.5	235.7	240.0	244.5	249.2	254.1
Temp. (K)	420						
c ($J K^{-1} g^{-1}$)	2.157						
C ($J K^{-1} mol^{-1}$)	259.2						

TABLE 14.32.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	71	30	0.820	8.15–2	0.31	–1.48–2	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
230.0–423.6	637.25	–6.63746	9.50896–1	1.36631+1	1.15827+1		III



Name: Naphthalene
Formula: $C_{10}H_8$

CAS–RN: 91–20–3
Group No.: 14–033
Molar Mass: 128.17

TABLE 14.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*90PIC		353.0–372.0	2	4.00	not specified	C_p	BDHO	*90PIC
26AND/LYN	N	354.0–473.0	eqn	nosp	not specified	C_p	DSIO	26AND/LYN
31BLA/LEI		382.0–465.8	17	3.00	not specified	C_{sat}	BSIO	31BLA/LEI
32SPA/THO		363.1–463.1	11S	1.00	not specified	C_p	BDHO	31THO/PAR
41SCH		353.0–473.0	eqn	nosp	not specified	C_p	not specified	
44EIB		353.0–473.0	eqn	nosp	not specified	C_p	not specified	
57MCC/FIN2		357.0–370.8	6	0.20	99.985 melpt	C_{sat}	BSAO	47HUF
64RAS/BAS		359.1	1	1.50	not specified	C_p	BSIO	64RAS/BAS
93DUR/AOU		373.0–473.0	102	nosp	not specified	C_p	BDCT	86MER/BEN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 14.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41SCH	353.0–472.7	10	0.50#	0.645	8.48–2	0.32	–4.45–2	–2
57MCC/FIN2	357.0–370.8	6	0.20	0.329	1.75–2	0.07	1.20–2	3
				Rejected data				
*90PIC	(4.59, 14.76, 4.57, 2)		26AND/LYN	(8.43–1, 2.76, 8.02–1, 9)				
31BLA/LEI	(5.63, 15.84, 5.58, 17)		32SPA/THO	(7.33–1, 2.49, 7.29–1, 11)				
44EIB	(4.50–1, 1.62, –4.42–1, –10)		64RAS/BAS	(2.44, 8.48, 2.44, 1)				
93DUR/AOU	(8.54–1, 2.84, 5.93–1, 56)							

TABLE 14.33.3. Parameters of regression polynomial

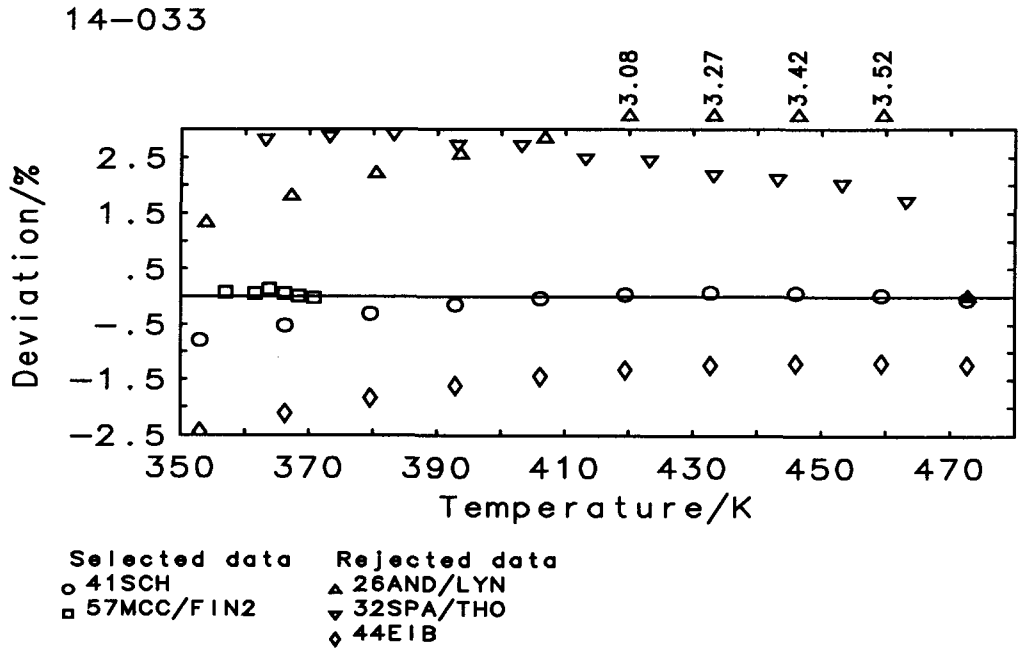
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C	169	16	0.608	7.54–2	0.29	−2.33–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
353.0–472.7		1.32901+1	2.51050	3.15992–1			III

TABLE 14.33.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c ($J K^{-1}g^{-1}$)	1.714	1.745	1.777	1.809	1.842	1.874	1.908
C ($J K^{-1}mol^{-1}$)	219.7	223.7	227.8	231.9	236.0	240.2	244.5
Temp. (K)	430	440	450	460	470		
c ($J K^{-1}g^{-1}$)	1.941	1.976	2.010	2.045	2.080		
C ($J K^{-1}mol^{-1}$)	248.8	253.2	257.6	262.1	266.6		

TABLE 14.33.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C	169	16	0.883	6.58–2	0.25	1.15–3	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
353.0–472.7	748.40	−3.43150	9.65806–2	9.26821	3.04803+1		III



Name: Tricyclo[3.3.2.0^{2,8}]deca–3,6,9–triene
Formula: $C_{10}H_{10}$

CAS-RN: 1005–51–2
Group No.: 14–034
Molar Mass: 130.19

TABLE 14.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FAL	N	380.0–450.0	8S	nosp	99.87	melpt	C_{sat}	BDHT	69PER/COM

80FAL *reproducibility given as 0.6–1.0 %*

TABLE 14.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.925	4.30–1	1.39	9.24–3	6
Temp. range K		A_1	A_2				Level of uncertainty
380.0–450.0		1.39771+1	4.34494				V

TABLE 14.34.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c_{sat} (J K^{-1}g^{-1})	1.95	1.97	2.00	2.03	2.06	2.09	2.11
C_{sat} (J K^{-1}mol^{-1})	253	257	261	264	268	272	275
Temp. (K)	450						
c_{sat} (J K^{-1}g^{-1})	2.14						
C_{sat} (J K^{-1}mol^{-1})	279						

Name: 1,2,3,4–Tetrahydronaphthalene
Formula: $C_{10}H_{12}$

CAS-RN: 119–64–2
Group No.: 14–035
Molar Mass: 132.21

TABLE 14.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
22HER/SCH	289.6	1	nosp	not specified		C_p	DSIO	22HER/SCH
57MCC/FIN2	248.4–318.5	11	0.20	99.97	melpt	C_{sat}	BSAO	47HUF

TABLE 14.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57MCC/FIN2	248.4–318.5	11	0.20	0.037	1.86–3	0.01	–1.04–6	–1
				Rejected data				
22HER/SCH	(1.14, 4.25, 1.14, 1)							

TABLE 14.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	11	0.047	2.33–3	0.01	–1.04–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
248.4–318.5		2.44682+1	–8.73212	4.50995	–4.66721–1		II

TABLE 14.35.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.480	1.512	1.546	1.557	1.580	1.616	1.645
C_{sat} (J K^{-1}mol^{-1})	195.7	200.0	204.4	205.8	209.0	213.6	217.5
Temp. (K)	300	310	320				
c_{sat} (J K^{-1}g^{-1})	1.652	1.688	1.724				
C_{sat} (J K^{-1}mol^{-1})	218.3	223.1	227.9				

TABLE 14.35.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	11	0.112	5.71–3	0.02	1.73–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
248.4–318.5	719.00	–1.18383+1	2.75198	9.82621	1.27314+1		II

Name: Butylbenzene
Formula: $C_{10}H_{14}$

CAS-RN: 104–51–8
Group No.: 14–036
Molar Mass: 134.22

TABLE 14.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31HUF/PAR	191.9–298.2	8	1.00	not specified		C_p	BSIO	25PAR
48TSC1	293.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC5	295.1	1	nosp	not specified		C_p	BSIO	48TSC1
65MES/TOD2	193.8–370.0	19	nosp	99.92	melpt	C_{sat}	BSAO	47HUF
83GRO/FAR3	298.1	1	0.30	99.	chrom	C_p	FSIT	71PIC/LED

TABLE 14.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65MES/TOD2	193.8–370.0	19	0.20#	0.063	3.61–3	0.01	–1.00–7	2
				Rejected data				
31HUF/PAR	(2.45–1, 0.87, –1.91–1, –7)			48TSC1	(3.72–1, 1.30, –3.72–1, –1)			
48TSC5	(3.42–1, 1.19, –3.42–1, –1)			83GRO/FAR3	(7.61–2, 0.26, –7.61–2, –1)			

TABLE 14.36.3. Parameters of regression polynomial

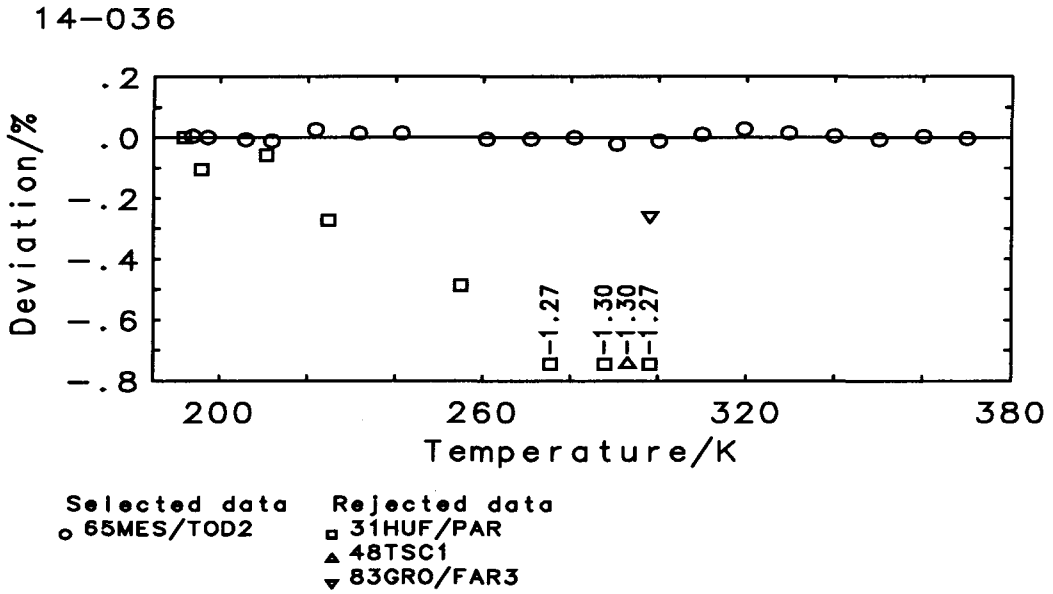
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	19	0.071	4.06–3	0.01	–1.00–7	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
193.8–370.0		3.30377+1	–1.24635+1	5.31326	–5.22035–1		II

TABLE 14.36.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J $K^{-1}g^{-1}$)	1.560	1.577	1.597	1.618	1.642	1.668	1.696
C_{sat} (J $K^{-1}mol^{-1}$)	209.4	211.7	214.3	217.2	220.4	223.9	227.6
Temp. (K)	270	273.15	280	290	298.15	300	
c_{sat} (J $K^{-1}g^{-1}$)	1.725	1.734	1.755	1.787	1.813	1.819	
C_{sat} (J $K^{-1}mol^{-1}$)	231.5	232.8	235.6	239.8	243.4	244.2	

TABLE 14.36.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	19	0.204	1.16–2	0.04	2.06–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
193.8–370.0	660.50	6.56869+2	6.94704+1	–4.58059+1	5.92385+2	2.03210+2	3.69694+2	II



Name: (1,1–Dimethylethyl)benzene
Formula: $C_{10}H_{14}$

CAS-RN: 98–06–6
Group No.: 14–037
Molar Mass: 134.22

TABLE 14.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
30HUF/PAR1	220.4–294.3	8	1.00	not specified		C_p	BSIO	25PAR

TABLE 14.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.195	5.23–2	0.19	1.34–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
220.4–294.3		2.55833+1	−3.80318	1.63987			IV

TABLE 14.37.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J\,K^{-1}g^{-1}$)	1.558	1.580	1.604	1.631	1.659	1.689	1.699
C_p ($J\,K^{-1}mol^{-1}$)	209.1	212.1	215.4	218.9	222.7	226.7	228.1
Temp. (K)	280	290	298.15				
c_p ($J\,K^{-1}g^{-1}$)	1.722	1.756	1.785				
C_p ($J\,K^{-1}mol^{-1}$)	231.1	235.7	239.6				

TABLE 14.37.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	8	8	0.178	4.79-2	0.18	1.08-4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
220.4-294.3	647.30	2.13126+1	2.17188+1	-6.76063-1	5.22848		IV

Name: 1-Methyl-4-(1-methylethyl)benzene
Formula: $C_{10}H_{14}$

CAS-RN: 99-87-6
Group No.: 14-038
Molar Mass: 134.22

TABLE 14.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	N	320.0-349.8	7S	nosp	not specified		C_{avg}	DSIO	*86SCH
31HUF/PAR		210.8-297.1	8	1.00	not specified		C_p	BSIO	25PAR
47KUR		305.9-358.5	4	nosp	not specified		C_{avg}	DSIO	47KUR

*86SCH substance not clearly identified, name "Cymen" used

TABLE 14.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
			Selected data					
*86SCH	320.0-349.8	7	1.00#	0.429	1.35-1	0.43	3.26-2	2
31HUF/PAR	210.8-297.1	8	1.00	0.271	7.49-2	0.27	-2.72-2	-2
			Rejected data					
47KUR	(3.28-1, 1.08, 1.83-2, -1)							

TABLE 14.38.3. Parameters of regression polynomial

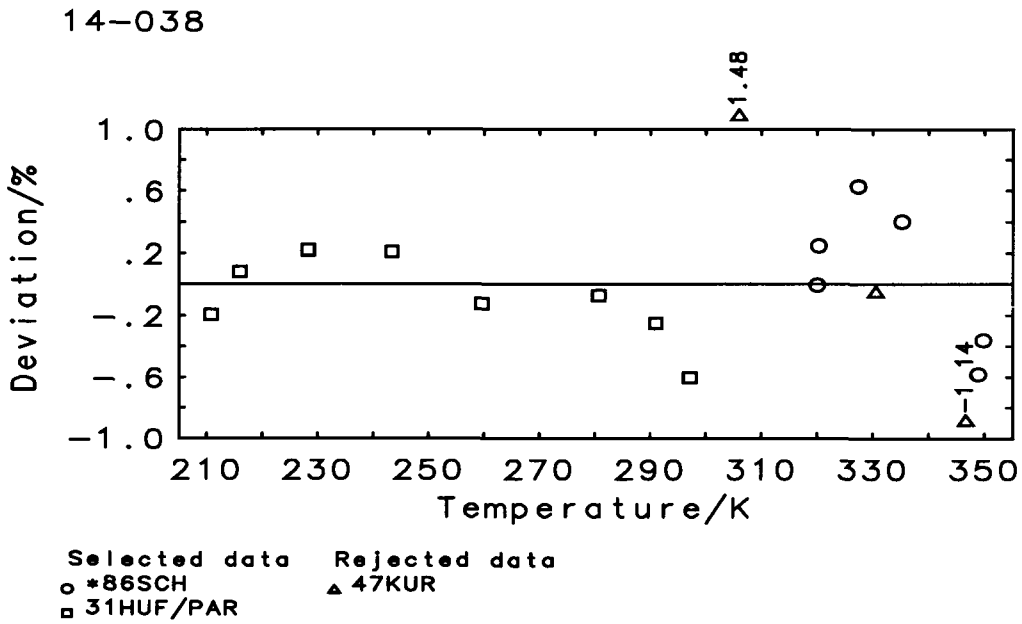
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	19	15	0.395	1.20-1	0.40	7.12-4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
210.8-349.8		2.90266+1	-6.49744	2.13944			IV

TABLE 14.38.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J\,K^{-1}g^{-1}$)	1.537	1.554	1.573	1.595	1.620	1.648	1.678
C_p ($J\,K^{-1}mol^{-1}$)	206.3	208.6	211.2	214.1	217.5	221.1	225.2
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	1.688	1.710	1.745	1.776	1.783	1.824	1.867
C_p ($J\,K^{-1}mol^{-1}$)	226.5	229.5	234.3	238.4	239.4	244.8	250.6
Temp. (K)	330	340	350				
c_p ($J\,K^{-1}g^{-1}$)	1.913	1.962	2.013				
C_p ($J\,K^{-1}mol^{-1}$)	256.8	263.3	270.2				

TABLE 14.38.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	15	0.473	1.43–1	0.47	–5.74–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
210.8–349.8	651.00	1.76135+1	1.99541+1	8.76667–1	3.88684		IV



Name: (1–Methylpropyl)benzene
Formula: $C_{10}H_{14}$

CAS-RN: 135–98–8
Group No.: 14–039
Molar Mass: 134.22

TABLE 14.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79AND/GRI	N	293.7–429.6	9	0.80	not specified		C_{sat}	BSAO	67RAS/GAN

79AND/GRI error 0.5 % below 373 K and 0.8 % at 433 K

TABLE 14.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.290	7.38–2	0.23	2.49–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
293.7–429.6		2.37272+1	–6.90785–1	8.58597–1			IV

TABLE 14.39.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.793	1.815	1.820	1.848	1.878	1.908	1.939
C_{sat} (J K^{-1}mol^{-1})	240.7	243.6	244.3	248.1	252.0	256.1	260.3
Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	1.972	2.005	2.040	2.075	2.112	2.150	2.188
C_{sat} (J K^{-1}mol^{-1})	264.6	269.1	273.8	278.5	283.5	288.5	293.7
Temp. (K)	420	430					
c_{sat} (J K^{-1}g^{-1})	2.228	2.269					
C_{sat} (J K^{-1}mol^{-1})	299.1	304.6					

TABLE 14.39.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.256	6.53–2	0.21	1.77–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
293.7–429.6	649.00	–7.73412	1.40394	1.70464+1	1.06516+1		IV

Name: 1,2,3,4–Tetramethylbenzene
Formula: $C_{10}H_{14}$

CAS-RN: 488–23–3
Group No.: 14–040
Molar Mass: 134.22

TABLE 14.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31HUF/PAR	276.5–291.9	4	1.00	not specified		C_p	BSIO	25PAR
47KUR	306.7–380.1	4	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 14.40.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31HUF/PAR	276.5–291.9	4	1.00	1.077	3.04–1	1.08	–5.64–2	0
47KUR	306.7–380.1	4	2.00#	0.613	3.77–1	1.23	2.63–1	2

TABLE 14.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	1.012	3.96–1	1.33	1.03–1	2

Temp. range K	A_1	A_2	Level of uncertainty
276.5–380.1	8.45928	6.97210	V

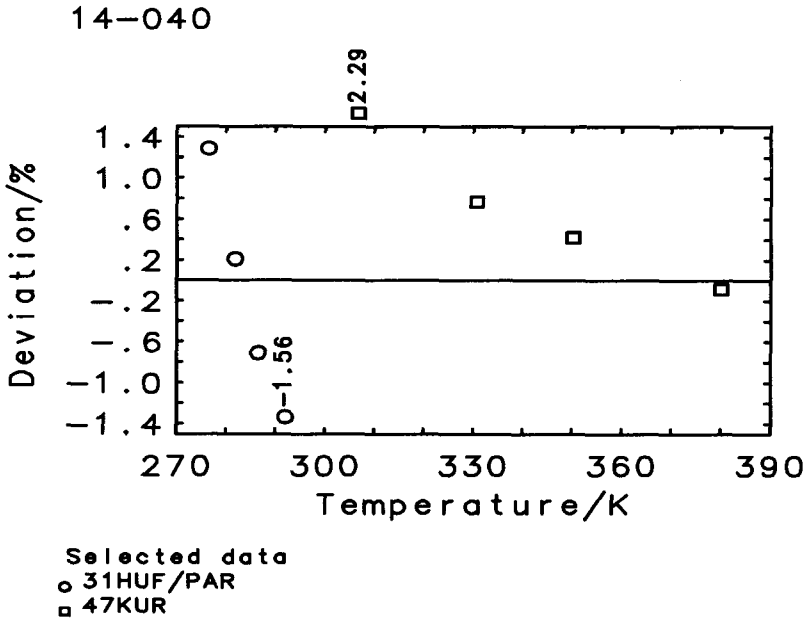
TABLE 14.40.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.73	1.78	1.81	1.82	1.86	1.91	1.95
C_p (J K^{-1}mol^{-1})	233	238	243	244	250	256	262
Temp. (K)	340	350	360	370	380		
c_p (J K^{-1}g^{-1})	1.99	2.04	2.08	2.12	2.17		
C_p (J K^{-1}mol^{-1})	267	273	279	285	291		

TABLE 14.40.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	1.087	4.81–1	1.59	1.10–1	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
276.5–380.1	689.70	–1.26889+1	2.91254	1.08890+1	1.38203+1	V



Name: 1,2,3,5–Tetramethylbenzene
Formula: $C_{10}H_{14}$

CAS-RN: 527–53–7
Group No.: 14–041
Molar Mass: 134.22

TABLE 14.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
31HUF/PAR	255.3–297.1	5	1.00	not specified	C_p	BSIO	25PAR

TABLE 14.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.113	3.20–2	0.11	5.19–5	1
Temp. range K		A_1	A_2				Level of uncertainty
255.3–297.1		1.60468+1	4.31873				IV

TABLE 14.41.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	1.690	1.716	1.725	1.743	1.770	1.792	1.797
C_p ($J\,K^{-1}mol^{-1}$)	226.8	230.4	231.5	234.0	237.6	240.5	241.1

Name: 1,2,4,5–Tetramethylbenzene
Formula: $C_{10}H_{14}$

CAS-RN: 95–93–2
Group No.: 14–042
Molar Mass: 134.22

TABLE 14.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
33FER/THO	363.1–393.1	4S	nosp	not specified		C_p	BDHO	31THO/PAR
44EIB	352.0–473.0	eqn	nosp	not specified		C_p	not specified	
47KUR	382.8–413.8	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 14.42.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33FER/THO	363.1–393.1	4	1.50#	1.104	5.55–1	1.65	5.54–1	4
44EIB	352.0–473.2	13	1.00#	0.297	9.71–2	0.30	–7.28–2	–9
				Rejected data				
47KUR	(2.07, 5.78, 2.06, 3)							

TABLE 14.42.3. Parameters of regression polynomial

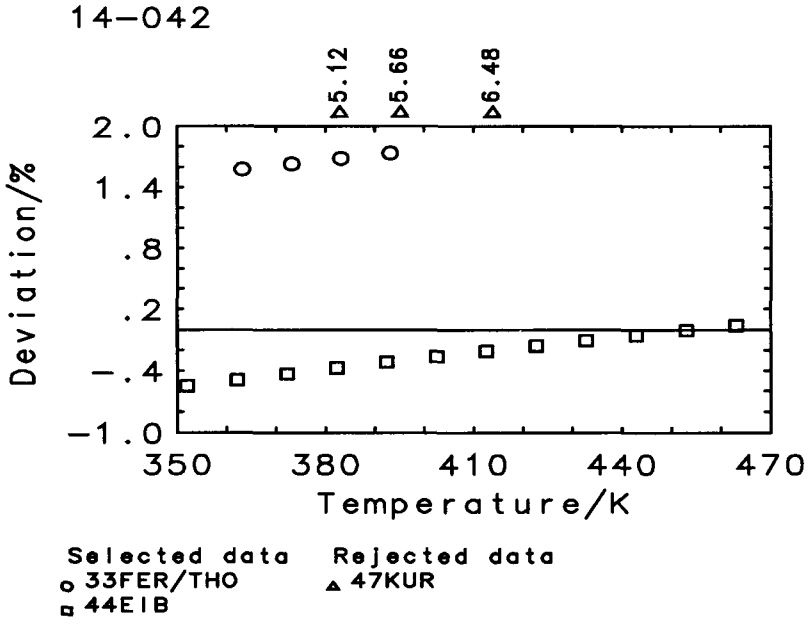
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	17	0.634	3.01–1	0.90	7.48–2	–5
Temp. range K		A_1	A_2				Level of uncertainty
352.0–473.2		1.85460+1	3.80813				V

TABLE 14.42.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c_p ($J\,K^{-1}g^{-1}$)	2.00	2.02	2.05	2.07	2.09	2.12	2.14
C_p ($J\,K^{-1}mol^{-1}$)	268	271	275	278	281	284	287
Temp. (K)	430	440	450	460	470		
c_p ($J\,K^{-1}g^{-1}$)	2.16	2.19	2.21	2.23	2.26		
C_p ($J\,K^{-1}mol^{-1}$)	290	294	297	300	303		

TABLE 14.42.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	17	0.782	3.00–1	0.91	–3.04–2	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
352.0–473.2	675.00	–1.90983	4.86320–2	2.09303+1	1.87502+1		V



Name: 1–Methyl–4–(1–methylethenyl)cyclohexene
Formula: $C_{10}H_{16}$

CAS-RN: 138–86–3
Group No.: 14–043
Molar Mass: 136.24

TABLE 14.43.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
33KOL/UDO	N	293.35	1.831	nosp	not specified		C_p	BSIT	34KOL/UDO2

33KOL/UDO same datum in 34KOL/UDO2

Name: 1–Methylnaphthalene
Formula: $C_{11}H_{10}$

CAS-RN: 90–12–0
Group No.: 14–044
Molar Mass: 142.20

TABLE 14.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57MCC/FIN2	248.0–352.2	15	0.20	99.95	melpt	C_{sat}	BSAO	47HUF

TABLE 14.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.064	3.52–3	0.01	1.91–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
248.0–352.2	3.24344+1	−1.43371+1	6.05156	−6.22299−1	II

TABLE 14.44.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.444	1.469	1.496	1.505	1.525	1.554	1.578
C_{sat} (J K^{-1}mol^{-1})	205.3	208.9	212.8	214.0	216.8	220.9	224.4
Temp. (K)	300	310	320	330	340	350	
c_{sat} (J K^{-1}g^{-1})	1.584	1.614	1.645	1.676	1.706	1.737	
C_{sat} (J K^{-1}mol^{-1})	225.2	229.5	233.9	238.3	242.7	247.0	

TABLE 14.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.354	1.91–2	0.07	2.20–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
248.0–352.2	772.00	–1.16043+1	2.59766	1.20903+1	1.29597+1		II

Name: 2-Methylnaphthalene
Formula: $C_{11}H_{10}$

CAS-RN: 91-57-6
Group No.: 14-045
Molar Mass: 142.20

TABLE 14.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31HUF/PAR	310.4	1	1.00	not specified		C_p	BSIO	25PAR
57MCC/FIN2	312.1–366.6	9	0.20	99.99	melpt	C_{sat}	BSAO	47HUF

TABLE 14.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31HUF/PAR	310.4	1	1.00	0.336	9.21–2	0.34	–9.21–2	–1
57MCC/FIN2	312.1–366.6	9	0.20	0.165	9.23–3	0.03	4.22–4	–1

TABLE 14.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	10	10	0.211	3.40–2	0.12	–8.83–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
310.4–366.6		1.20537+1	4.97583				II

TABLE 14.45.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c ($J K^{-1}g^{-1}$)	1.607	1.636	1.665	1.694	1.723	1.752	1.781
C ($J K^{-1}mol^{-1}$)	228.5	232.6	236.7	240.9	245.0	249.2	253.3

Name: 1,1–Dimethylindan
Formula: $C_{11}H_{14}$

CAS-RN: 4912–92–9
Group No.: 14–046
Molar Mass: 146.23

TABLE 14.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEE/FIN	236.0–388.8	20	0.20	99.914	melpt	C_{sat}	BSAO	47HUF

TABLE 14.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.159	9.51–3	0.03	4.86–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
236.0–388.8	2.37687+1	–3.85559	2.66628	–2.25518–1	II

TABLE 14.46.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} ($J K^{-1}g^{-1}$)	1.521	1.551	1.581	1.612	1.622	1.645	1.678
C_{sat} ($J K^{-1}mol^{-1}$)	222.5	226.7	231.2	235.8	237.2	240.5	245.4
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} ($J K^{-1}g^{-1}$)	1.706	1.712	1.747	1.782	1.818	1.855	1.891
C_{sat} ($J K^{-1}mol^{-1}$)	249.4	250.3	255.4	260.6	265.9	271.2	276.6
Temp. (K)	360	370	380	390			
c_{sat} ($J K^{-1}g^{-1}$)	1.929	1.966	2.004	2.042			
C_{sat} ($J K^{-1}mol^{-1}$)	282.0	287.5	293.0	298.6			

Name: 4,6–Dimethylindan
Formula: $C_{11}H_{14}$

CAS-RN: 1685–82–1
Group No.: 14–047
Molar Mass: 146.23

TABLE 14.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEE/FIN	262.0–370.5	12	0.20	99.992	melpt	C_{sat}	BSAO	47HUF

TABLE 14.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.395	2.30–2	0.08	2.04–5	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
262.0–370.5		1.89140+1	1.16774	7.42060–1			II

TABLE 14.47.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.533	1.562	1.572	1.592	1.623	1.648	1.654
C_{sat} (J K^{-1}mol^{-1})	224.2	228.5	229.8	232.8	237.3	241.1	241.9
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	1.687	1.720	1.754	1.789	1.825	1.861	1.899
C_{sat} (J K^{-1}mol^{-1})	246.7	251.5	256.5	261.6	266.8	272.2	277.7

Name: 4,7–Dimethylindan
Formula: $C_{11}H_{14}$

CAS-RN: 6682–71–9
Group No.: 14–048
Molar Mass: 146.23

TABLE 14.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81LEE/FIN	285.8–393.9	11	0.20	99.984	melpt	C_{sat}	BSAO	47HUF

TABLE 14.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.293	1.88–2	0.06	3.29–6	–2
Temp. range K		A_1	A_2				Level of uncertainty
285.8–393.9		1.14135+1	5.91154				II

TABLE 14.48.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.624	1.651	1.657	1.691	1.725	1.758	1.792
C_{sat} (J K^{-1}mol^{-1})	237.4	241.4	242.4	247.3	252.2	257.1	262.0
Temp. (K)	350	360	370	380	390		
c_{sat} (J K^{-1}g^{-1})	1.825	1.859	1.893	1.926	1.960		
C_{sat} (J K^{-1}mol^{-1})	266.9	271.8	276.8	281.7	286.6		

Name: Pentamethylbenzene
Formula: $C_{11}H_{16}$

CAS-RN: 700–12–9
Group No.: 14–049
Molar Mass: 148.25

TABLE 14.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
33FER/THO	333.1–393.1	7S	nosp	not specified	C_p	BDHO	31THO/PAR
44EIB	328.0–473.0	eqn	nosp	not specified	C_p	not specified	

TABLE 14.49.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
44EIB	328.0–473.6	15	1.00#	0.000	2.41–6	0.00	5.09–7	0
				Rejected data				
33FER/THO	(8.34–1, 2.26, 6.53–1, 5)							

TABLE 14.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	15	0.000	2.59–6	0.00	5.09–7	0
Temp. range K		A_1	A_2				Level of uncertainty
328.0–473.6		2.35673+1	3.17054				V

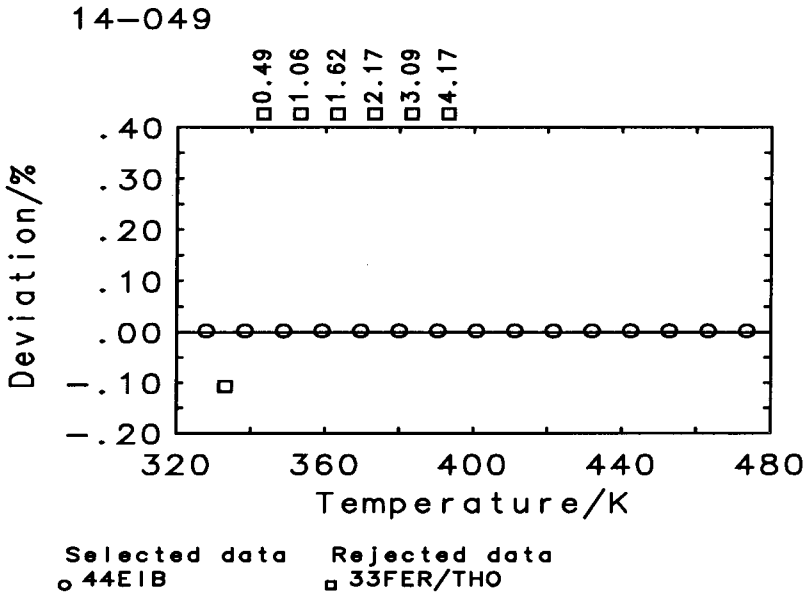
TABLE 14.49.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	1.91	1.93	1.94	1.96	1.98	2.00	2.02
C_p ($J K^{-1} mol^{-1}$)	283	286	288	291	293	296	299
Temp. (K)	400	410	420	430	440	450	460
c_p ($J K^{-1} g^{-1}$)	2.03	2.05	2.07	2.09	2.10	2.12	2.14
C_p ($J K^{-1} mol^{-1}$)	301	304	307	309	312	315	317
Temp. (K)	470						
c_p ($J K^{-1} g^{-1}$)	2.16						
C_p ($J K^{-1} mol^{-1}$)	320						

TABLE 14.49.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	22	15	0.000	2.91-6	0.00	-1.78-6	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
328.0–473.6	719.00	-7.88201-5	6.8132-11	2.35673+1	2.27960+1	V



Name: Acenaphthylene
Formula: $C_{12}H_8$

CAS-RN: 208-96-8
Group No.: 14-050
Molar Mass: 152.20

TABLE 14.50.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
69SAD/STE	N	393.15	1.093	nosp	not specified		C_{avg}	DSIO	69SAD/STE

69SAD/STE average value in temperature range 363–423 K; possible decomposition at higher temperatures

Name: Acenaphthene
Formula: $C_{12}H_{10}$

CAS-RN: 83-32-9
Group No.: 14-051
Molar Mass: 154.21

TABLE 14.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
35SKA	N	367.0–377.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN
44EIB		368.0–473.0	eqn	nosp	not specified		C_p	not specified	
69SAD/STE		366.0–473.0	eqn	nosp	not specified		C_p	DSIO	69SAD/STE
77FIN/MES		374.2–436.4	10	0.20	99.981	melpt	C_{sat}	BSAO	47HUF

35SKA temperature range not specified, recommended use near n.m.t.

TABLE 14.51.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
77FIN/MES	374.2–436.4	10	0.20	0.374	2.49–2	0.07	3.74–5	3
				Rejected data				
35SKA	(5.91–1, 1.80, 5.91–1, 1)			44EIB	(4.12, 10.93, 4.11, 5)			
69SAD/STE	(5.52, 13.68, 5.32, 9)							

TABLE 14.51.3. Parameters of regression polynomial

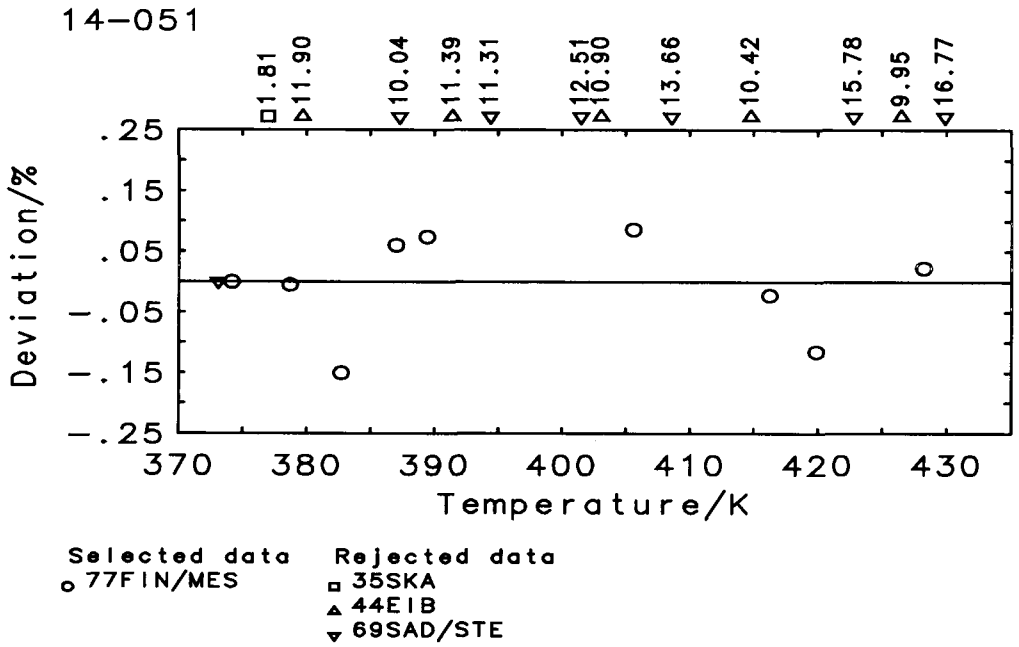
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	38	10	0.419	2.79–2	0.08	3.74–5	3
Temp. range K		A_1	A_2				Level of uncertainty
374.2–436.4		1.06600+1	5.70431				II

TABLE 14.51.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420
c_{sat} ($J K^{-1} g^{-1}$)	1.743	1.774	1.805	1.836	1.866
C_{sat} ($J K^{-1} mol^{-1}$)	268.9	273.6	278.3	283.1	287.8

TABLE 14.51.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	38	10	0.447	2.98–2	0.09	3.78–5	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
374.2–436.4	803.20	–3.26683–1	5.90845–4	1.07623+1	4.51563+1		II



Name: 1,1'–Biphenyl
Formula: $C_{12}H_{10}$

CAS-RN: 92–52–4
Group No.: 14–052
Molar Mass: 154.21

TABLE 14.52.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type Reference
31FOR/BRU		350.8–469.6	22	2.00	not specified	C_p	BSIO 31FOR/BRU
31FOR/BRU		420.8–620.2	8	2.00	not specified	C_p	FSIO 31FOR/BRU
31NEW/KAU	N	344.0–573.0	eqn	1.00	not specified	C_p	not specified
32SPA/THO		353.1–373.1	3S	nosp	not specified	C_p	BDHO 31THO/PAR
41SCH		342.0–473.0	eqn	nosp	not specified	C_p	not specified
50KUR		386.4–492.8	10	nosp	not specified	C_{avg}	DSIO 47KUR
56MCE/MAL		422.0–588.7	4S	nosp	not specified	C_p	not specified
58WAL/BRO		429.8–533.3	3	2.00	not specified	C_p	DSIO 56WAL/GRA
83ORO/MRA		350.0–480.0	24S	1.50	99.9 chrom	C_p	BDHT 69PER/COM
89CHI/KNI		349.1–440.3	11	0.10	99.983 melpt	C_{sat}	BSAO 47HUF
89CHI/KNI		360.0–700.0	18	1.00	99.983 melpt	C_{sat}	BDHT 89KNI/ARC
93DUR/AOU		373.0–473.0	51	nosp	not specified	C_p	BDCT 86MER/BEN

31NEW/KAU four different calorimeters used

TABLE 14.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89CHI/KNI	349.1–440.3	11	0.10	0.190	6.56–3	0.02	–1.51–3	–3
89CHI/KNI	360.0–700.0	18	1.00#	0.680	2.87–1	0.68	9.64–2	4
				Rejected data				
31FOR/BRU	(1.41, 3.67, 3.33–1, –2)			31FOR/BRU	(4.11, 8.43, 3.54, 6)			
31NEW/KAU	(5.52–1, 1.36, –2.39–1, –3)			32SPA/THO	(1.64–1, 0.50, –1.41–1, –3)			
41SCH	(4.39–1, 1.20, –7.05–2, –1)			50KUR	(2.30, 5.86, 1.95, 10)			
56MCE/MAL	(9.51–1, 2.10, 6.21–1, 2)			58WAL/BRO	(1.98–1, 0.49, –2.98–2, –1)			
83ORO/MRA	(3.23–1, 0.89, –2.12–1, –12)			93DUR/AOU	(1.39, 3.85, –1.23, –51)			

TABLE 14.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	174	29	0.591	2.43–1	0.58	5.92–2	1
C_{sat}	174	29	0.557	2.23–1	0.54	6.18–2	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
349.1–700.0		1.61319+1	4.17889	2.29446–1	–1.72138–2		IV
349.1–700.0		1.82988+1	2.60244	6.08539–1	–4.73438–2		IV

TABLE 14.52.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	1.770	1.798	1.826	1.854	1.882	1.910	1.938
C_p (J K^{-1}mol^{-1})	273.0	277.3	281.6	285.9	290.2	294.5	298.8
c_{sat} (J K^{-1}g^{-1})	1.770	1.798	1.826	1.854	1.881	1.909	1.938
C_{sat} (J K^{-1}mol^{-1})	273.0	277.3	281.5	285.8	290.1	294.5	298.8
Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	1.966	1.994	2.022	2.050	2.078	2.106	2.134
C_p (J K^{-1}mol^{-1})	303.1	307.4	311.8	316.1	320.4	324.7	329.0
c_{sat} (J K^{-1}g^{-1})	1.966	1.994	2.022	2.050	2.078	2.106	2.134
C_{sat} (J K^{-1}mol^{-1})	303.1	307.4	311.8	316.1	320.4	324.7	329.1
Temp. (K)	490	500	510	520	530	540	550
c_p (J K^{-1}g^{-1})	2.162	2.190	2.218	2.245	2.273	2.301	2.329
C_p (J K^{-1}mol^{-1})	333.3	337.7	342.0	346.3	350.6	354.8	359.1
c_{sat} (J K^{-1}g^{-1})	2.162	2.189	2.217	2.245	2.272	2.299	2.326
C_{sat} (J K^{-1}mol^{-1})	333.3	337.6	341.9	346.1	350.4	354.5	358.7
Temp. (K)	560	570	580	590	600	610	620
c_p (J K^{-1}g^{-1})	2.356	2.384	2.412	2.439	2.467	2.494	2.521
C_p (J K^{-1}mol^{-1})	363.4	367.7	371.9	376.1	380.4	384.6	388.8
c_{sat} (J K^{-1}g^{-1})	2.353	2.380	2.406	2.432	2.458	2.484	2.509
C_{sat} (J K^{-1}mol^{-1})	362.9	367.0	371.1	375.1	379.1	383.1	387.0

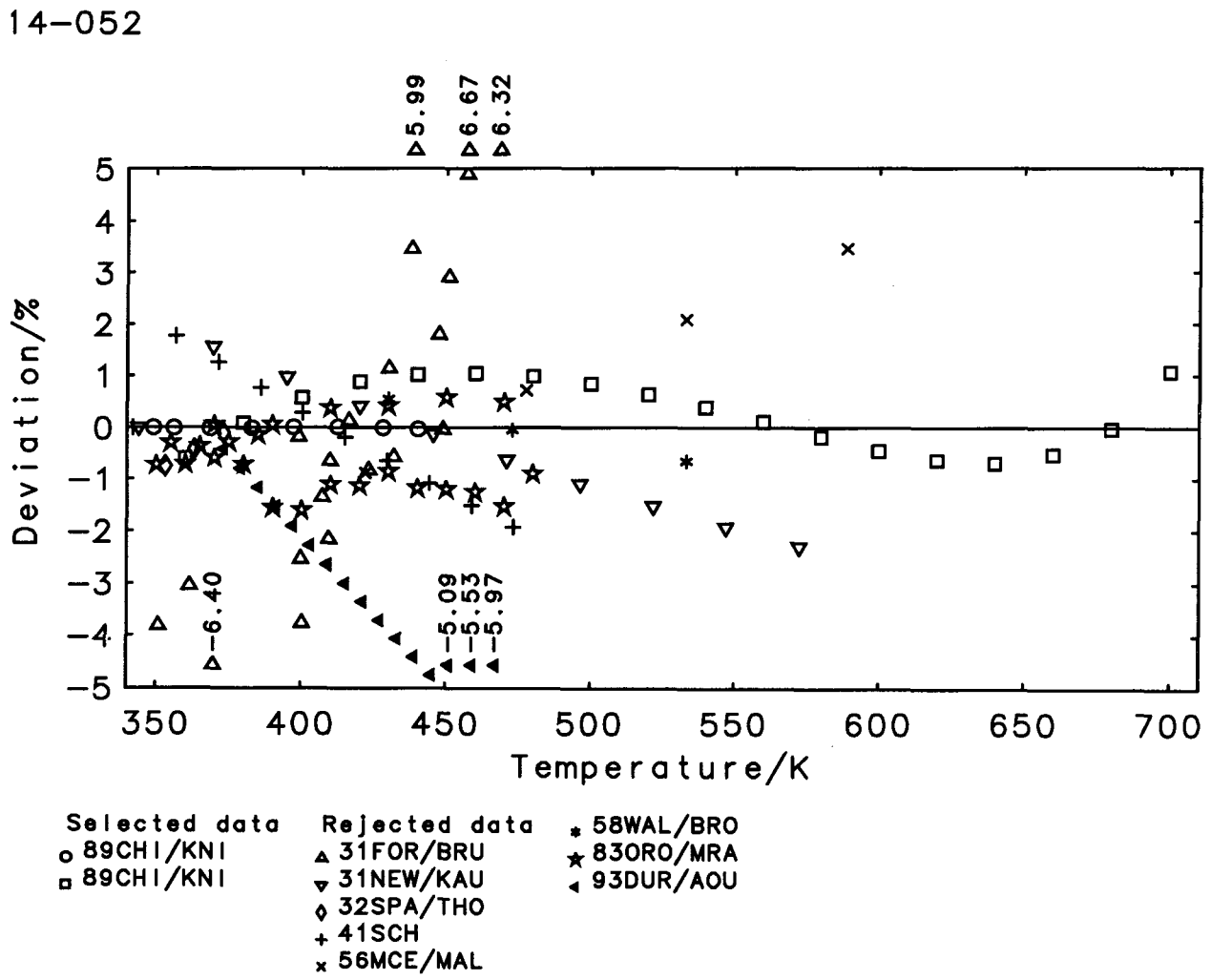
TABLE 14.52.4. Recommended values of heat capacities (continued)

Temp. (K)	630	640	650	660	670	680	690
c_p ($J K^{-1}g^{-1}$)	2.548	2.575	2.602	2.629	2.656	2.682	2.709
C_p ($J K^{-1}mol^{-1}$)	393.0	397.1	401.3	405.4	409.5	413.6	417.7
c_{sat} ($J K^{-1}g^{-1}$)	2.535	2.559	2.584	2.608	2.632	2.655	2.678
C_{sat} ($J K^{-1}mol^{-1}$)	390.9	394.7	398.5	402.2	405.9	409.5	413.0

Temp. (K)	700
c_p ($J K^{-1}g^{-1}$)	2.735
C_p ($J K^{-1}mol^{-1}$)	421.7
c_{sat} ($J K^{-1}g^{-1}$)	2.701
C_{sat} ($J K^{-1}mol^{-1}$)	416.5

TABLE 14.52.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	174	29	1.253	2.42–1	0.54	–2.85–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
349.1–700.0	780.00	1.33336	1.00099–2	1.36467+1	4.44026+1		IV



Name: 1,8–Dimethylnaphthalene
Formula: $C_{12}H_{12}$

CAS-RN: 569–41–5
Group No.: 14–053
Molar Mass: 156.23

TABLE 14.53.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
77FIN/MES	349.6–432.3	7	0.20	99.9955	melpt	C_{sat}	BSAO	47HUF

TABLE 14.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.265	1.91–2	0.05	–8.72–6	1

Temp. range K	A_1	A_2	Level of uncertainty
349.6–432.4	1.22890+1	6.09189	II

TABLE 14.53.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	1.789	1.821	1.854	1.886	1.918	1.951	1.983
C_{sat} (J K^{-1}mol^{-1})	279.5	284.5	289.6	294.7	299.7	304.8	309.8

Temp. (K)	420	430
c_{sat} (J K^{-1}g^{-1})	2.016	2.048
C_{sat} (J K^{-1}mol^{-1})	314.9	320.0

TABLE 14.53.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.204	1.53–2	0.04	7.08–6	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
349.6–432.4	792.00	6.38062	1.69089–1	1.04137+1	6.01934+1	II

Name: 2,3–Dimethylnaphthalene
Formula: $C_{12}H_{12}$

CAS-RN: 581–40–8
Group No.: 14–054
Molar Mass: 156.23

TABLE 14.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88MES/FIN	384.5–415.1	8	0.10	99.935	melpt	C_{sat}	BSAO	47HUF

TABLE 14.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.706	2.58–2	0.07	2.43–5	–4
Temp. range K		A_1	A_2				Level of uncertainty
384.5–415.1		1.49680+1	5.41211				II

TABLE 14.54.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	1.891	1.920	1.949	1.978
C_{sat} (J K^{-1}mol^{-1})	295.4	299.9	304.4	308.9

Name: 2,6–Dimethylnaphthalene
Formula: $C_{12}H_{12}$

CAS-RN: 581–42–0
Group No.: 14–055
Molar Mass: 156.23

TABLE 14.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77FIN/MES	390.2–438.3	9	0.20	99.958	melpt	C_{sat}	BSAO	47HUF

TABLE 14.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.646	4.88–2	0.13	1.12–4	0
Temp. range K		A_1	A_2				Level of uncertainty
390.2–438.3		1.19193+1	6.00463				II

TABLE 14.55.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440
c_{sat} (J K^{-1}g^{-1})	1.881	1.913	1.945	1.977	2.009	2.040
C_{sat} (J K^{-1}mol^{-1})	293.8	298.8	303.8	308.8	313.8	318.8

Name: 2,7–Dimethylnaphthalene
Formula: $C_{12}H_{12}$

CAS-RN: 582–16–1
Group No.: 14–056
Molar Mass: 156.23

TABLE 14.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77FIN/MES	372.6–391.0	6	0.20	99.95	melpt	C_{sat}	BSAO	47HUF

TABLE 14.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	6	6	0.469	3.27–2	0.09	4.13–5	0
Temp. range K		A_1	A_2				Level of uncertainty
372.6–391.0		1.25511+1	5.87490				II

TABLE 14.56.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_{sat} (J K^{-1}g^{-1})	1.825	1.856	1.887
C_{sat} (J K^{-1}mol^{-1})	285.1	290.0	294.9

Name: Cyclohexylbenzene
Formula: $C_{12}H_{16}$

CAS-RN: 827–52–1
Group No.: 14–057
Molar Mass: 160.26

TABLE 14.57.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83ORO/MRA	290.0–470.0	37S	1.00	99.9	chrom	C_p	BDHT	69PER/COM

TABLE 14.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	37	0.905	3.34–1	0.91	5.13–3	–1 0
Temp. range K		A_1	A_2				Level of uncertainty
290.0–470.0		9.23013	7.50904				V

TABLE 14.57.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.61	1.64	1.65	1.69	1.73	1.76	1.80
C_p (J K^{-1}mol^{-1})	258	263	264	270	277	283	289
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	1.84	1.88	1.92	1.96	2.00	2.04	2.08
C_p (J K^{-1}mol^{-1})	295	302	308	314	320	326	333
Temp. (K)	420	430	440	450	460	470	
c_p (J K^{-1}g^{-1})	2.12	2.15	2.19	2.23	2.27	2.31	
C_p (J K^{-1}mol^{-1})	339	345	351	358	364	370	

TABLE 14.57.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	37	0.908	3.35–1	0.91	5.50–3	–9
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
290.0–470.0	742.00	6.03820	1.35392–1	7.40096	6.73228+1		V

Name: *E,E,Z*–1,5,9–Cyclododecatriene
Formula: $C_{12}H_{18}$

CAS-RN: 706–31–0
Group No.: 14–058
Molar Mass: 162.27

TABLE 14.58.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
89LAI/ROD	298.15	1.773	nosp	99.	anal	C_p	FSIT	71PIC/LED

Name: Hexamethylbenzene
Formula: $C_{12}H_{18}$

CAS-RN: 87–85–4
Group No.: 14–059
Molar Mass: 162.27

TABLE 14.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
32SPA/THO	443.1–473.1	4S	1.00	not specified		C_p	BDHO	31THO/PAR
47KUR	470.3–492.6	2	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 14.59.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
32SPA/THO	443.1–473.1	4	1.00	0.039	1.83–2	0.04	1.24–5	0
				Rejected data				
47KUR	(1.97, 4.31, –1.97, –1)							

TABLE 14.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	4	0.055	2.58–2	0.06	1.24–5	0
Temp. range K		A_1	A_2				Level of uncertainty
443.1–473.1		6.97009	8.65599				V

TABLE 14.59.4. Recommended values of heat capacities

Temp. (K)	440	450	460	470
c_p ($J\,K^{-1}g^{-1}$)	2.31	2.35	2.40	2.44
C_p ($J\,K^{-1}mol^{-1}$)	375	382	389	396

Name: Hexylbenzene
Formula: $C_{12}H_{18}$

CAS-RN: 1077–16–3
Group No.: 14–060
Molar Mass: 162.27

TABLE 14.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48TSC1	293.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC5	295.1	1	nosp	not specified		C_p	BSIO	48TSC1

TABLE 14.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
293.1–295.1	5.92153+1	–8.16594	VI

TABLE 14.60.4. Recommended values of heat capacities

Temp. (K)	293	295
c_p ($J\,K^{-1}g^{-1}$)	1.81	1.80
C_p ($J\,K^{-1}mol^{-1}$)	293	292

Name: 9*H*–Fluorene
Formula: $C_{13}H_{10}$

CAS-RN: 86–73–7
Group No.: 14–061
Molar Mass: 166.22

TABLE 14.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
44EIB	387.0–473.0	eqn	nosp	not specified		C_p	not specified	
77FIN/MES	392.6–426.7	8	0.20	99.992	melpt	C_{sat}	BSAO	47HUF

TABLE 14.61.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
44EIB	387.0–472.0	18	1.00#	0.611	2.16–1	0.61	–1.16–1	–3
77FIN/MES	392.6–426.7	8	0.20	0.348	2.54–2	0.07	1.08–2	3

TABLE 14.61.3. Parameters of regression polynomial

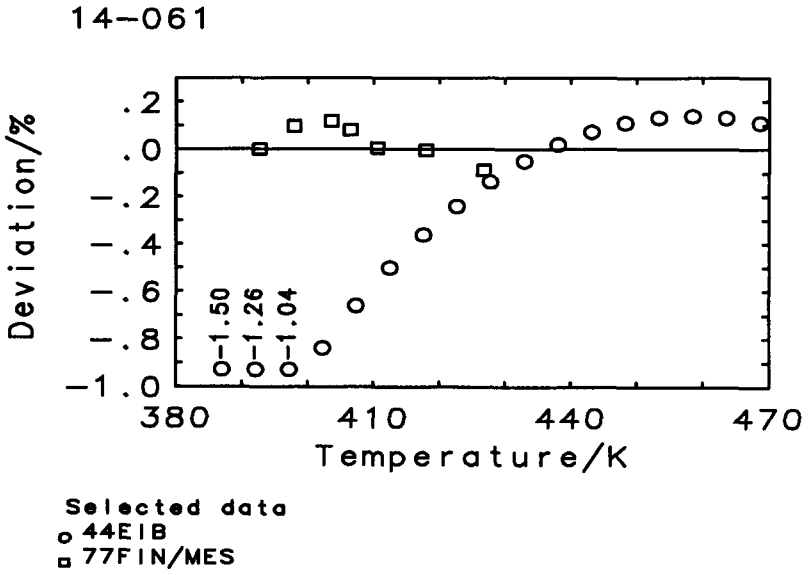
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	26	26	0.578	1.92–1	0.54	–7.74–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
387.0–472.0		3.10273+1	–3.23336	1.12314			III

TABLE 14.61.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440	450
c ($J K^{-1} g^{-1}$)	1.776	1.804	1.833	1.864	1.895	1.928	1.962
C ($J K^{-1} mol^{-1}$)	295.2	299.9	304.7	309.8	315.0	320.5	326.1
Temp. (K)	460	470					
c ($J K^{-1} g^{-1}$)	1.997	2.033					
C ($J K^{-1} mol^{-1}$)	331.9	337.9					

TABLE 14.61.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	26	26	1.447	1.33–1	0.37	4.42–3	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
387.0–472.0	825.00	–1.04989+1	9.11211–1	1.24839+1	3.02420+1		III



Name: 1,1'–Methylenebisbenzene
Formula: $C_{13}H_{12}$

CAS-RN: 101–81–5
Group No.: 14–062
Molar Mass: 168.24

TABLE 14.62.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30HUF/PAR1		302.0–312.3	4	nosp	not specified		C_p	BSIO	25PAR
31BLA/LEI		308.1–368.1	13	nosp	not specified		C_p	BSIO	31BLA/LEI
31SMI/AND1		310.7–322.6	2	nosp	99.9	estim	C_p	DSIO	26AND/LYN
50KUR		313.8–414.4	8	nosp	not specified		C_{avg}	DSIO	47KUR
56DUF/EVE	N	303.1–353.1	6S	nosp	not specified		C_p	not specified	

56DUF/EVE measured by a non–calorimetric method (piezo–thermometric)

TABLE 14.62.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
30HUF/PAR1	302.0–312.3	4	1.00#	0.363	1.17–1	0.36	1.08–1	4
56DUF/EVE	303.1–353.1	6	0.50#	0.305	5.03–2	0.15	–1.78–2	–2
			Rejected data					
31BLA/LEI	(3.52, 9.43, 3.43, 10)		31SMI/AND1	(4.90–1, 1.48, 4.50–1, 2)				
50KUR	(2.41, 6.70, 2.40, 4)							

TABLE 14.62.3. Parameters of regression polynomial

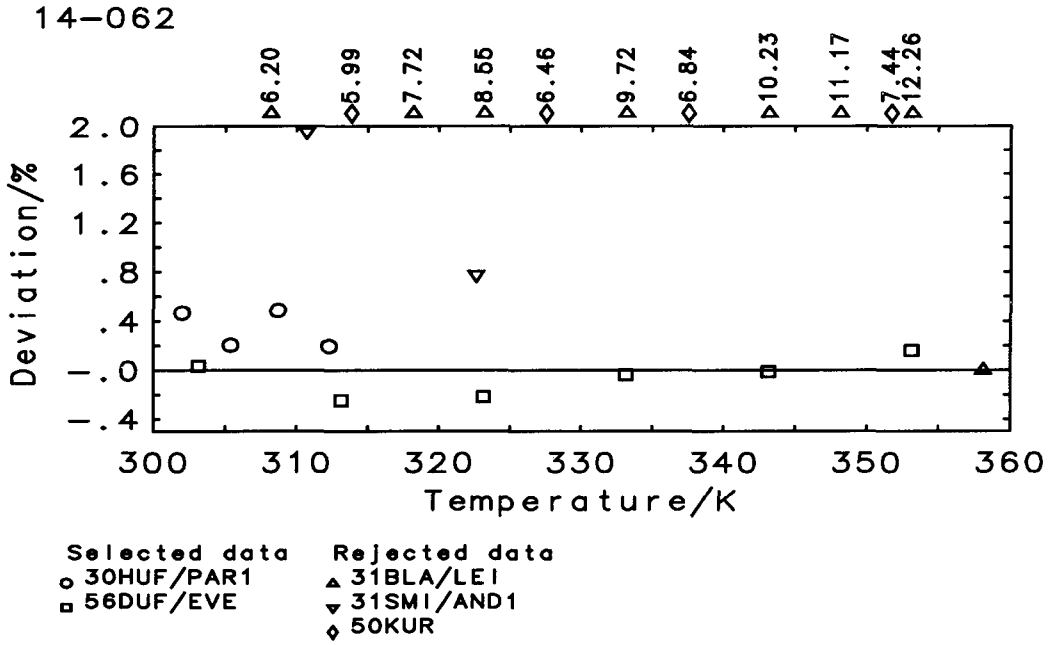
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	10	0.368	9.36–2	0.29	3.28–2	2
Temp. range K		A_1	A_2				Level of uncertainty
302.0–353.1		1.70065+1	4.94395				III

TABLE 14.62.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.573	1.598	1.622	1.647	1.671	1.696
C_p ($J\,K^{-1}mol^{-1}$)	264.7	268.8	272.9	277.1	281.2	285.3

TABLE 14.62.5. Parameters of quasi–polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	10	0.329	7.15–2	0.22	8.34–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
302.0–353.1	770.00	6.04128+1	3.94115+1	–1.18128+1	2.31513+1		III



Name: 1,1,4,6–Tetramethylindan
Formula: $C_{13}H_{18}$

CAS-RN: 941–60–6
Group No.: 14–063
Molar Mass: 174.29

TABLE 14.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEE/FIN	286.1–377.6	12	0.20	99.937	melpt	C_{sat}	BSAO	47HUF

TABLE 14.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.295	2.25–2	0.06	–5.40–6	2
Temp. range K		A_1	A_2				Level of uncertainty
286.1–377.6		1.35539+1	7.53843				II

TABLE 14.63.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.690	1.719	1.725	1.761	1.797	1.833	1.869
C_{sat} (J K^{-1}mol^{-1})	294.5	299.6	300.7	307.0	313.3	319.5	325.8
Temp. (K)	350	360	370	380			
c_{sat} (J K^{-1}g^{-1})	1.905	1.941	1.977	2.013			
C_{sat} (J K^{-1}mol^{-1})	332.1	338.3	344.6	350.9			

Name: 1,1,4,7–Tetramethylindan
Formula: $C_{13}H_{18}$

CAS-RN: 1078–04–2
Group No.: 14–064
Molar Mass: 174.29

TABLE 14.64.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEE/FIN	170.1–376.4	20	0.20	99.67	melpt	C_{sat}	BSAO	47HUF

TABLE 14.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.263	1.74–2	0.05	1.55–5	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
170.1–376.4		3.05143+1	–6.97221	4.25614	–4.21718–1		II

TABLE 14.64.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.378	1.398	1.419	1.442	1.466	1.492	1.520
C_{sat} (J K^{-1}mol^{-1})	240.2	243.6	247.3	251.3	255.6	260.1	264.9
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.549	1.579	1.610	1.642	1.652	1.675	1.708
C_{sat} (J K^{-1}mol^{-1})	269.9	275.2	280.6	286.2	287.9	291.9	297.7
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.736	1.742	1.777	1.811	1.846	1.881	1.916
C_{sat} (J K^{-1}mol^{-1})	302.5	303.6	309.6	315.7	321.8	327.9	334.0
Temp. (K)	360	370	380				
c_{sat} (J K^{-1}g^{-1})	1.951	1.986	2.020				
C_{sat} (J K^{-1}mol^{-1})	340.0	346.1	352.0				

Name: Heptylbenzene
Formula: $C_{13}H_{20}$

CAS-RN: 1078–71–3
Group No.: 14–065
Molar Mass: 176.30

TABLE 14.65.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48TSC1	294.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC5	295.1	1	nosp	not specified		C_p	BSIO	48TSC1

TABLE 14.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
294.1–295.1	3.87698+1	VI

TABLE 14.65.4. Recommended values of heat capacities

Temp. (K)	294	295
c_p ($J K^{-1} g^{-1}$)	1.83	1.83
C_p ($J K^{-1} mol^{-1}$)	322	322

Name: Anthracene
Formula: $C_{14}H_{10}$

CAS-RN: 120–12–7
Group No.: 14–066
Molar Mass: 178.23

TABLE 14.66.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
17HIL/DUS	N	526.2–541.2	2	nosp	not specified	C_{avg}	DSIO	11LEW/RAN
70GOU/GIR	N	496.7–511.3	5	0.10	99.99 melpt	C_{sat}	BSAO	53WES/HAT
93DUR/AOU		492.0–592.0	51	nosp	not specified	C_p	BD*CT*	86MER/BEN

17HIL/DUS average values in temperature ranges 489–563 K and 489–593 K
70GOU/GIR smoothed value at 500 K in 68GOU/GIR

TABLE 14.66.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
17HIL/DUS	526.2–541.2	2	3.00#	0.229	3.17–1	0.69	1.80–1	0
70GOU/GIR	496.7–511.3	5	0.10	3.920	1.75–1	0.39	4.20–3	–1
93DUR/AOU	492.0–592.0	51	3.00#	0.403	5.34–1	1.21	–2.43–1	–7

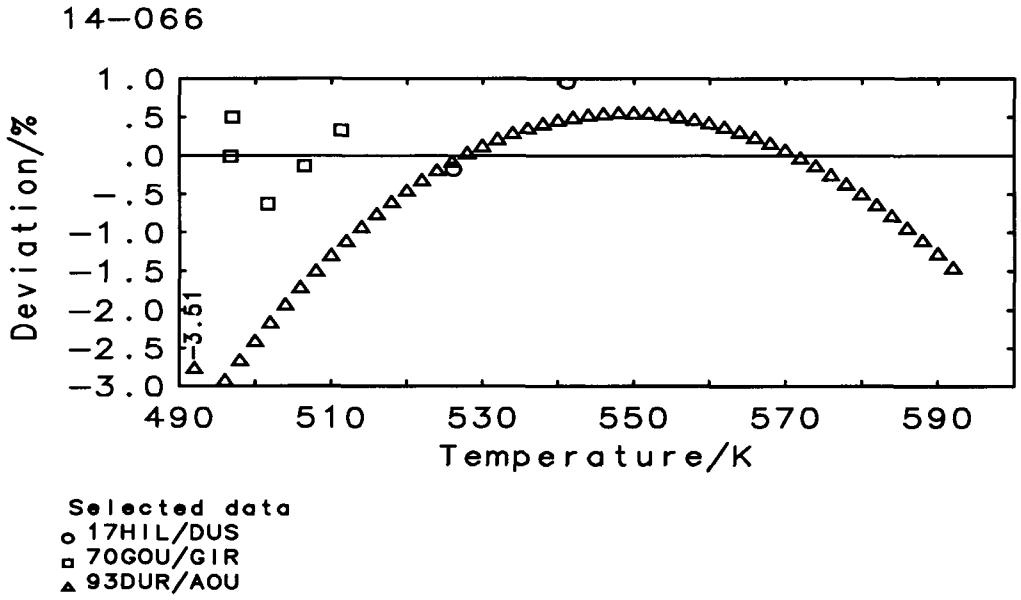
TABLE 14.66.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	58	58	1.245	5.21–1	1.18	–2.07–1	–8

Temp. range K	A_1	A_2	A_3	Level of uncertainty
492.0–592.0	1.74875+2	–5.28183+1	5.35102	V

TABLE 14.66.4. Recommended values of heat capacities

Temp. (K)	490	500	510	520	530	540	550
c ($J K^{-1} g^{-1}$)	2.08	2.08	2.08	2.10	2.11	2.13	2.16
C ($J K^{-1} mol^{-1}$)	370	370	372	373	376	380	384
Temp. (K)	560	570	580	590			
c ($J K^{-1} g^{-1}$)	2.19	2.22	2.26	2.31			
C ($J K^{-1} mol^{-1}$)	390	396	404	412			



Name: 1,1'–(1,2–Ethynediyl)bisbenzene
Formula: $C_{14}H_{10}$

CAS-RN: 501–65–5
Group No.: 14–067
Molar Mass: 178.23

TABLE 14.67.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50KUR	364.5–552.5	10	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 14.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	10	10	0.265	4.65–1	1.06	8.84–3	4
Temp. range K		A_1	A_2				Level of uncertainty
364.5–552.5		1.23024+1	6.88427				VI

TABLE 14.67.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c ($J K^{-1} g^{-1}$)	1.76	1.79	1.83	1.86	1.89	1.92	1.95
C ($J K^{-1} mol^{-1}$)	314	320	326	331	337	343	348
Temp. (K)	440	450	460	470	480	490	500
c ($J K^{-1} g^{-1}$)	1.99	2.02	2.05	2.08	2.12	2.15	2.18
C ($J K^{-1} mol^{-1}$)	354	360	366	371	377	383	388
Temp. (K)	510	520	530	540	550		
c ($J K^{-1} g^{-1}$)	2.21	2.24	2.28	2.31	2.34		
C ($J K^{-1} mol^{-1}$)	394	400	406	411	417		

Name: Phenanthrene
Formula: $C_{14}H_{10}$

CAS-RN: 85–01–8
Group No.: 14–068
Molar Mass: 178.23

TABLE 14.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type Reference
41SCH	371.0–473.0	eqn	nosp	not specified	C_p	not specified
44EIB	371.0–473.0	eqn	nosp	not specified	C_p	not specified
64RAS/BAS	379.1	1	1.50	not specified	C_p	BSIO 64RAS/BAS
77FIN/MES	383.3–408.6	4	0.20	99.987 melpt	C_{sat}	BSAO 47HUF
93DUR/AOU	392.0–492.0	51	nosp	not specified	C_p	BDCT 86MER/BEN

TABLE 14.68.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41SCH	371.0–472.7	10	1.00#	0.758	3.07–1	0.76	9.97–3	–4
77FIN/MES	383.3–408.6	4	0.20	0.084	6.38–3	0.02	–4.16–3	–2
93DUR/AOU	392.0–492.0	51	2.00#	0.383	2.97–1	0.77	3.30–2	–13
				Rejected data				
44EIB	(1.04, 2.79, –3.55–1, –4)			64RAS/BAS	(1.55+1, 29.80, 1.55+1, 1)			

TABLE 14.68.3. Parameters of regression polynomial

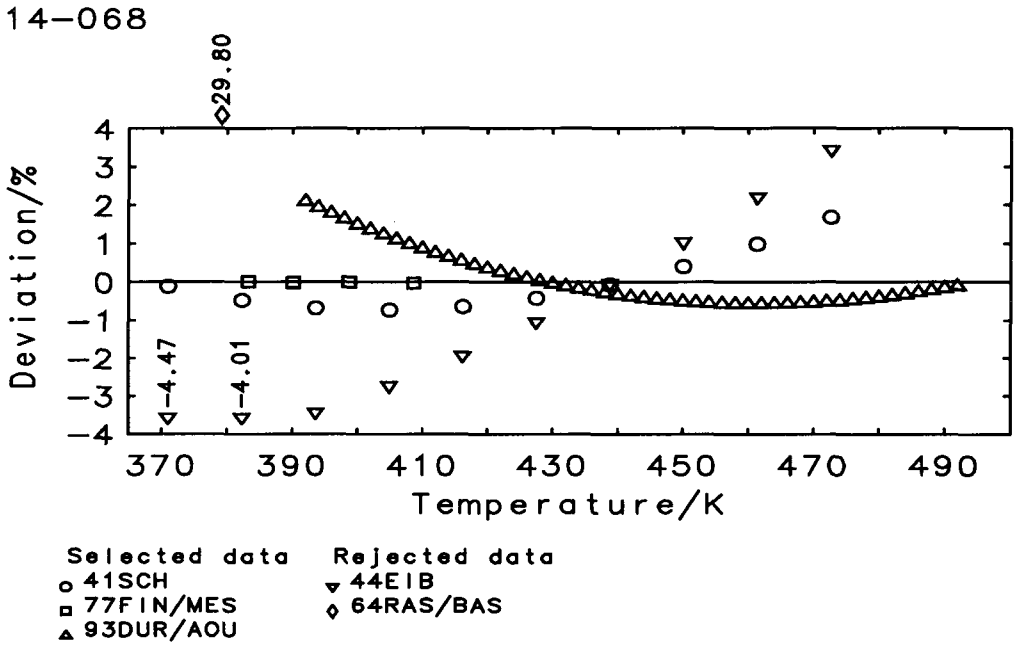
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	76	65	0.462	2.96–1	0.76	2.72–2	–19
Temp. range K		A_1	A_2	A_3			Level of uncertainty
371.0–492.0		–2.07752+1	2.30443+1	–2.09945			V

TABLE 14.68.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c ($J K^{-1} g^{-1}$)	1.70	1.73	1.76	1.79	1.82	1.84	1.86
C ($J K^{-1} mol^{-1}$)	303	309	314	319	324	328	332
Temp. (K)	450	460	470	480	490		
c ($J K^{-1} g^{-1}$)	1.89	1.90	1.92	1.93	1.95		
C ($J K^{-1} mol^{-1}$)	336	339	342	345	347		

TABLE 14.68.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	76	65	1.392	2.78–1	0.72	–4.99–2	–17
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
371.0–492.0	873.00	2.69250+2	4.70347+1	–6.02175+1	3.85330+2		V



Name: 9,10–Dihydrophenanthrene
Formula: $C_{14}H_{12}$

CAS-RN: 776–35–2
Group No.: 14–069
Molar Mass: 180.25

TABLE 14.69.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79LEE/HOS	310.2–349.5	34	0.20	99.75	melpt	C_{sat}	BSAO	47HUF

TABLE 14.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	34	0.968	6.75–2	0.19	2.50–4	1
Temp. range K		A_1	A_2				Level of uncertainty
310.2–349.5		1.44190+1	6.43817				II

TABLE 14.69.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.586	1.615	1.645	1.675	1.705
C_{sat} (J K^{-1}mol^{-1})	285.8	291.2	296.5	301.9	307.2

Name: (*E*)–1,1'–(1,2–Ethenediyl)bisbenzene
Formula: $C_{14}H_{12}$

CAS-RN: 103–30–0
Group No.: 14–070
Molar Mass: 180.25

TABLE 14.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33FER/THO	403.1	1	nosp	not specified		C_p	BDHO	31THO/PAR
50KUR	449.3–552.9	6	nosp	not specified		C_{avg}	DSIO	47KUR
85BOU/DEL	401.6–410.6	4	nosp	99.95	melpt	C_p	BSAO	85BOU/DEL

TABLE 14.70.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50KUR	449.3–552.9	6	3.00#	0.366	4.92–1	1.10	–2.38–1	–1
85BOU/DEL	401.6–410.6	4	0.30#	0.325	4.18–2	0.10	3.83–3	0
				Rejected data				
33FER/THO	(3.60–1, 0.85, –3.60–1, –1)							

TABLE 14.70.3. Parameters of regression polynomial

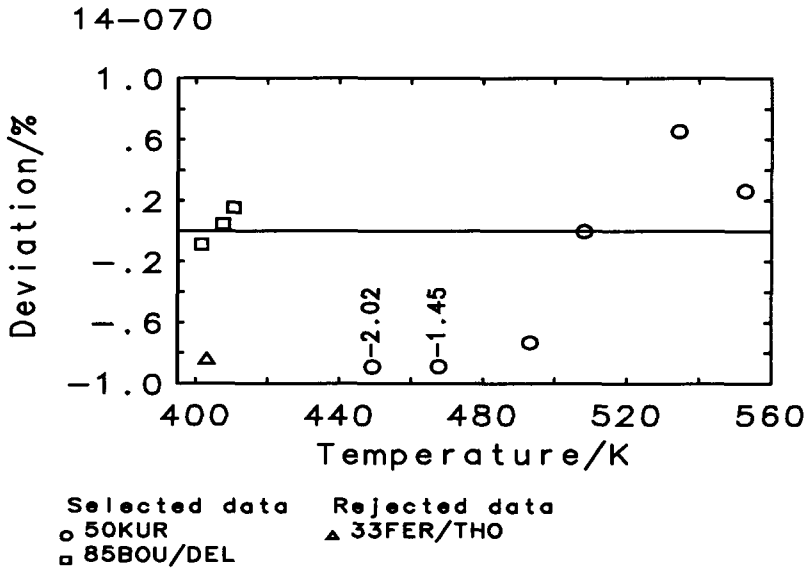
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	10	0.418	4.57–1	1.02	–1.42–1	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
401.6–552.9		3.57797+1	–9.26465–1	6.51152–1			V

TABLE 14.70.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450	460
c_p (J K^{-1}g^{-1})	1.96	1.98	2.00	2.02	2.04	2.07	2.09
C_p (J K^{-1}mol^{-1})	353	357	361	364	368	372	377
Temp. (K)	470	480	490	500	510	520	530
c_p (J K^{-1}g^{-1})	2.11	2.14	2.16	2.19	2.21	2.24	2.27
C_p (J K^{-1}mol^{-1})	381	385	390	394	399	404	409
Temp. (K)	540	550					
c_p (J K^{-1}g^{-1})	2.30	2.32					
C_p (J K^{-1}mol^{-1})	414	419					

TABLE 14.70.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	10	4.261	5.99–1	1.39	2.08–1	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
401.6–552.9	819.00	–9.52009	1.25421	2.40722+1	1.80656+1		V



Name: 1,1'–Ethenylidenebisbenzene
Formula: $C_{14}H_{12}$

CAS-RN: 530–48–3
Group No.: 14–071
Molar Mass: 180.25

TABLE 14.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31SMI/AND1	286.0–298.5	2	nosp	99.3	melpt	C_p	DSIO	26AND/LYN

TABLE 14.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
286.0–298.5		1.91565+1	5.63602				V

TABLE 14.71.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.64	1.66	1.66
C_p ($J K^{-1} mol^{-1}$)	295	299	300

Name: 1,1'–(1,2–Ethanediyl)bisbenzene
Formula: $C_{14}H_{14}$

CAS-RN: 103–29–7
Group No.: 14–072
Molar Mass: 182.27

TABLE 14.72.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
08BOG/WIN N	348.1	1	nosp	not specified	C_{avg}	DSIO	08BOG/WIN
33FER/THO	333.1–343.1	2S	nosp	not specified	C_p	BDHO	31THO/PAR
41SCH	324.0–473.0	eqn	nosp	not specified	C_p	not specified	
50KUR	349.4–427.4	5	nosp	not specified	C_{avg}	DSIO	47KUR
88MES/FIN	335.3–372.3	15	0.10	99.961 melpt	C_{sat}	BSAO	47HUF

08BOG/WIN average value in temperature range 325–371 K

TABLE 14.72.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41SCH	324.0–472.4	15	1.50#	0.528	3.16–1	0.79	1.10–2	–5
88MES/FIN	335.3–372.3	15	0.10	0.627	2.49–2	0.06	7.38–6	0
				Rejected data				
08BOG/WIN	(1.31, 3.23, 1.31, 1)		33FER/THO	(9.53–2, 0.25, 9.50–2, 2)				
50KUR	(9.08–1, 2.08, 8.78–1, 5)							

TABLE 14.72.3. Parameters of regression polynomial

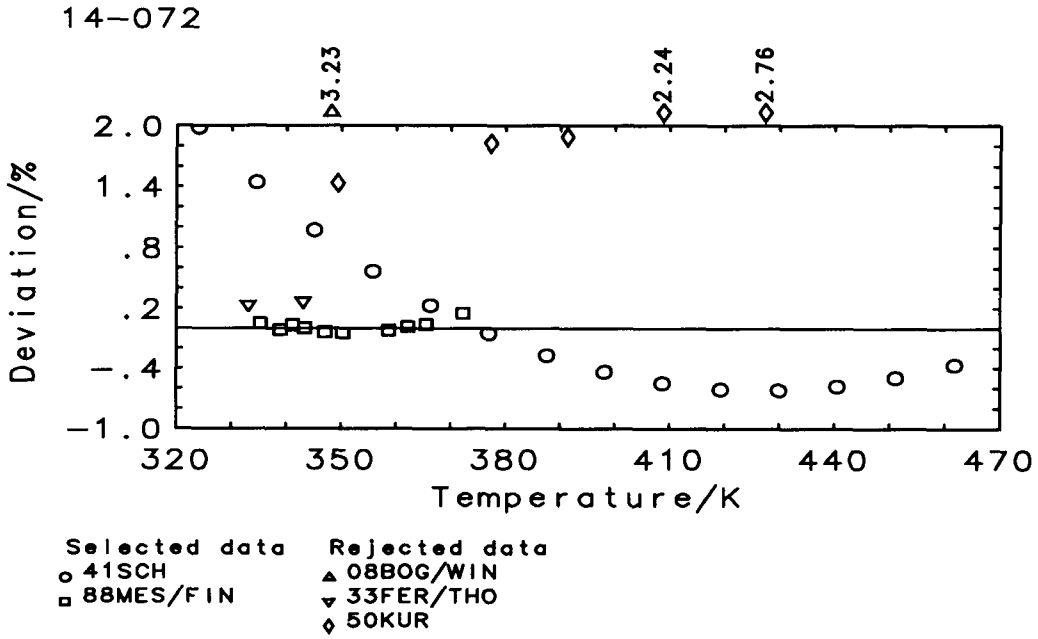
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	38	30	0.611	2.36–1	0.59	5.48–3	–5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
324.0–472.4		3.42711	1.35622+1	–9.41607–1			III

TABLE 14.72.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c ($J K^{-1}g^{-1}$)	1.730	1.763	1.796	1.827	1.857	1.887	1.916
C ($J K^{-1}mol^{-1}$)	315.4	321.4	327.3	333.0	338.5	343.9	349.2
Temp. (K)	400	410	420	430	440	450	460
c ($J K^{-1}g^{-1}$)	1.944	1.971	1.997	2.022	2.047	2.071	2.093
C ($J K^{-1}mol^{-1}$)	354.3	359.2	364.0	368.6	373.1	377.4	381.5
Temp. (K)	470						
c ($J K^{-1}g^{-1}$)	2.115						
C ($J K^{-1}mol^{-1}$)	385.5						

TABLE 14.72.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_h/R	+/–
C	38	30	4.572	1.91–1	0.49	–7.50–2	–9
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
324.0–472.4	785.00	8.62970	3.07069–1	1.70449+1	6.06311+1		III



Name: 1,1'–Ethylidenebisbenzene
Formula: $C_{14}H_{14}$

CAS-RN: 612–00–0
Group No.: 14–073
Molar Mass: 182.27

TABLE 14.73.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31SMI/AND1	259.8–298.5	4	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 14.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.132	8.87–2	0.26	1.98–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
259.8–298.5		1.43694+1	7.08295				V

TABLE 14.73.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.50	1.53	1.54	1.56	1.59	1.62	1.62
C_p ($J K^{-1} mol^{-1}$)	273	278	280	284	290	295	296

Name: 1,2,3,4,5,6,7,8–Octahydroanthracene
Formula: $C_{14}H_{18}$

CAS-RN: 1079–71–6
Group No.: 14–074
Molar Mass: 186.30

TABLE 14.74.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71BOY/SAN	372.0–390.0	2	nosp	99.9	melpt	C_p	BDHT	73PER/COM
82GAM/CAL	351.6–396.1	10	0.05	99.996	melpt	C_{sat}	BSAO	47HUF

TABLE 14.74.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82GAM/CAL	351.6–396.1	10	0.05	0.241	5.10–3	0.01	1.53–6	0
				Rejected data				
71BOY/SAN	(3.08, 6.60, 3.05, 2)							

TABLE 14.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	10	0.289	6.10–3	0.01	1.53–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
351.6–396.1		–7.68131	1.87469+1	–1.40580			II

TABLE 14.74.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400
c_{sat} ($J K^{-1} g^{-1}$)	1.817	1.856	1.894	1.931	1.966	2.000
C_{sat} ($J K^{-1} mol^{-1}$)	338.5	345.8	352.8	359.7	366.2	372.6

Name: Octylbenzene
Formula: $C_{14}H_{22}$

CAS-RN: 2189–60–8
Group No.: 14–075
Molar Mass: 190.33

TABLE 14.75.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48TSC1	295.1	1	nosp	not specified		C_p	BSIO	48TSC1
48TSC5	295.1	1	nosp	not specified		C_p	BSIO	48TSC1

TABLE 14.75.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.158	2.03–1	0.48	9.65–4	0
Temp. range K		A_1					Level of uncertainty
295.1–295.1		4.27633+1					V

TABLE 14.75.4. Recommended values of heat capacities

Temp. (K)	295.1
c_p ($J K^{-1} g^{-1}$)	1.87
C_p ($J K^{-1} mol^{-1}$)	356

Name: 4–Methylphenanthrene
Formula: $C_{15}H_{12}$

CAS-RN: 832–64–4
Group No.: 14–076
Molar Mass: 192.26

TABLE 14.76.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89CHI/HOS	331.7–445.3	18	nosp	99.92	melpt	C_{sat}	BSAO	47HUF

TABLE 14.76.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.275	1.09–2	0.03	6.78–6	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
331.7–445.3		7.10016	1.00294+1	−3.43111–1			II

TABLE 14.76.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	1.577	1.610	1.643	1.676	1.709	1.741	1.773
C_{sat} (J K^{-1}mol^{-1})	303.2	309.6	316.0	322.3	328.5	334.7	340.9
Temp. (K)	400	410	420	430	440		
c_{sat} (J K^{-1}g^{-1})	1.805	1.836	1.867	1.898	1.928		
C_{sat} (J K^{-1}mol^{-1})	346.9	353.0	358.9	364.9	370.7		

TABLE 14.76.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.264	1.04–2	0.03	5.51–6	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
331.7–445.3	898.60	2.23454+1	1.22605	7.36100	1.01814+2		II

Name: (1–Methylethyl)–1,1'–biphenyl
Formula: $C_{15}H_{16}$

CAS-RN: 25640–78–2
Group No.: 14–077
Molar Mass: 196.29

TABLE 14.77.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
56MCE/MAL		422.0–588.7	4S	nosp	not specified	C_p	not specified	
63VAR/KOP	N	293.1–671.2	10	1.50	not specified	C_{sat}	BSAO	63VAR/KOP
64VUK/RAS		311.8–485.0	6	3.00	not specified	C_{sat}	BDHO	64VUK/RAS

63VAR/KOP maximum difference between reported values (measured at 1 MPa) for C_{sat} is 0.5 %

TABLE 14.77.2. Correlated heat capacities

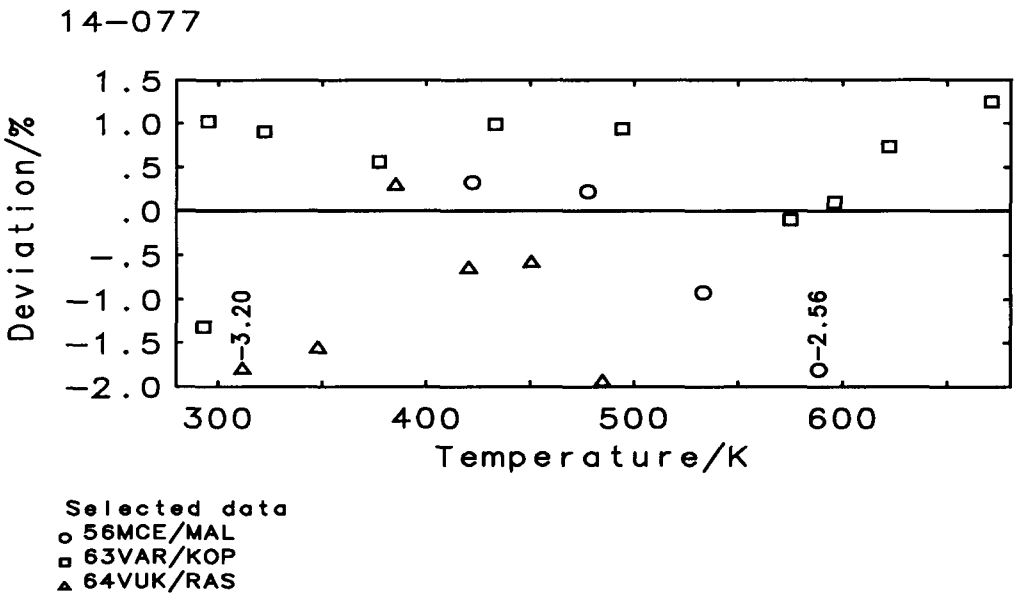
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56MCE/MAL	422.0–588.7	4	1.50#	0.916	8.84–1	1.37	–4.84–1	0
63VAR/KOP	293.1–671.2	10	1.50	0.591	4.96–1	0.89	3.08–1	6
64VUK/RAS	311.8–485.0	6	3.00	0.567	7.73–1	1.70	–5.97–1	–4

TABLE 14.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	20	20	0.719	7.34–1	1.39	–1.22–1	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
293.1–671.2		3.08238+1	1.01804	8.63981–1			V

TABLE 14.77.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c ($J K^{-1} g^{-1}$)	1.74	1.76	1.76	1.79	1.82	1.85	1.88
C ($J K^{-1} mol^{-1}$)	341	345	346	352	357	362	368
Temp. (K)	350	360	370	380	390	400	410
c ($J K^{-1} g^{-1}$)	1.90	1.94	1.97	2.00	2.03	2.06	2.10
C ($J K^{-1} mol^{-1}$)	374	380	386	392	399	405	412
Temp. (K)	420	430	440	450	460	470	480
c ($J K^{-1} g^{-1}$)	2.13	2.17	2.20	2.24	2.28	2.32	2.36
C ($J K^{-1} mol^{-1}$)	419	426	433	440	447	455	462
Temp. (K)	490	500	510	520	530	540	550
c ($J K^{-1} g^{-1}$)	2.40	2.44	2.48	2.52	2.56	2.61	2.65
C ($J K^{-1} mol^{-1}$)	470	478	486	495	503	511	520
Temp. (K)	560	570	580	590	600	610	620
c ($J K^{-1} g^{-1}$)	2.69	2.74	2.79	2.83	2.88	2.93	2.98
C ($J K^{-1} mol^{-1}$)	529	538	547	556	566	575	585
Temp. (K)	630	640	650	660	670		
c ($J K^{-1} g^{-1}$)	3.03	3.08	3.13	3.18	3.24		
C ($J K^{-1} mol^{-1}$)	595	605	615	625	635		



Name: Fluoranthene
Formula: $C_{16}H_{10}$

CAS-RN: 206-44-0
Group No.: 14-078
Molar Mass: 202.26

TABLE 14.78.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71WON/WES	393.7–422.6	5	0.10	99.936	melpt	C_{sat}	BSAO	68WES/WES
71WON/WES	386.4–451.7	10	0.10	99.61	melpt	C_{sat}	BSAO	68WES/WES
93DUR/AOU	492.0–592.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 14.78.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71WON/WES	393.7–422.6	5	0.10	3.557	1.53–1	0.36	9.50–2	4
71WON/WES	386.4–451.7	10	0.10	1.821	7.64–2	0.18	–4.68–2	–6

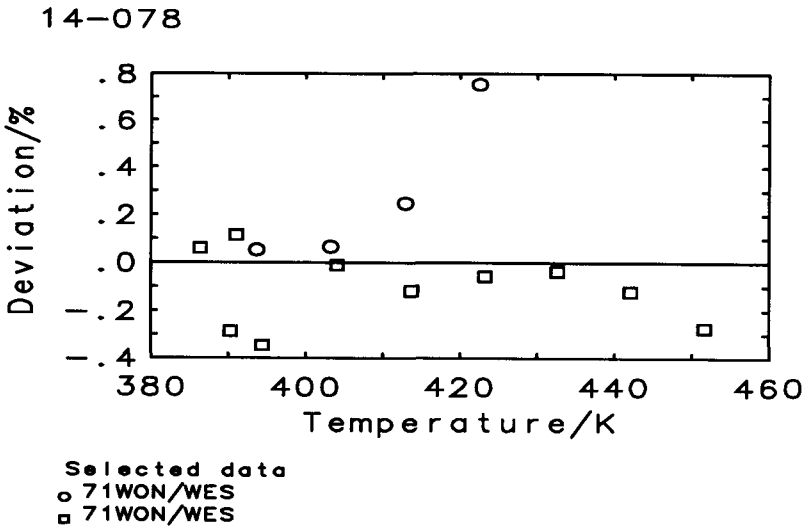
TABLE 14.78.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	66	15	2.724	1.16–1	0.27	5.05–4	–2

Temp. range K	A_1	A_2	Level of uncertainty
386.4–451.7	1.42876+1	6.76896	II

TABLE 14.78.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	1.673	1.700	1.728	1.756	1.784	1.812	1.840
C_{sat} (J K^{-1}mol^{-1})	338.3	343.9	349.5	355.2	360.8	366.4	372.1



Name: Pyrene
Formula: $C_{16}H_{10}$

CAS-RN: 129-00-0
Group No.: 14-079
Molar Mass: 202.26

TABLE 14.79.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
71WON/WES	430.6–478.8	7	0.10	99.97 melpt	C_{sat}	BSAO	68WES/WES
93DUR/AOU	492.0–592.0	51	nosp	not specified	C_p	BDCT	86MER/BEN

TABLE 14.79.2. Correlated heat capacities

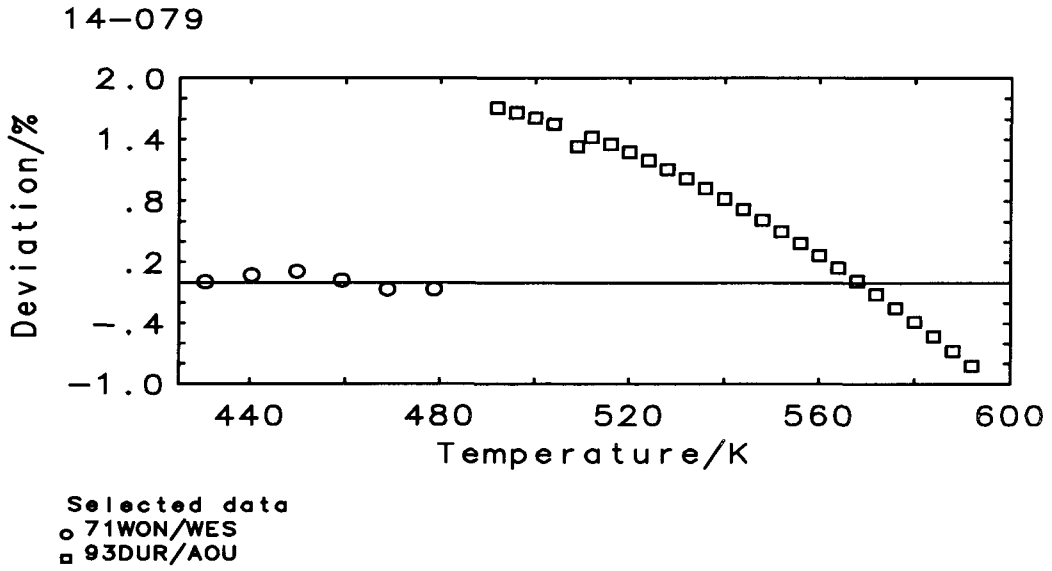
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71WON/WES	430.6–478.8	7	0.10	0.689	3.02–2	0.07	–2.45–3	0
93DUR/AOU	492.0–592.0	51	3.00#	0.333	4.92–1	01.00	3.18–1	27

TABLE 14.79.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	58	58	0.404	4.74–1	0.96	2.79–1	27
Temp. range K		A_1	A_2	A_3			Level of uncertainty
430.6–592.0		3.04330+1	–8.79318–1	8.49992–1			IV

TABLE 14.79.4. Recommended values of heat capacities

Temp. (K)	430	440	450	460	470	480	490
c ($J K^{-1}g^{-1}$)	1.742	1.769	1.796	1.824	1.853	1.883	1.913
C ($J K^{-1}mol^{-1}$)	352.3	357.7	363.2	368.9	374.8	380.8	386.9
Temp. (K)	500	510	520	530	540	550	560
c ($J K^{-1}g^{-1}$)	1.944	1.976	2.008	2.041	2.075	2.109	2.144
C ($J K^{-1}mol^{-1}$)	393.2	399.6	406.1	412.8	419.6	426.6	433.7
Temp. (K)	570	580	590				
c ($J K^{-1}g^{-1}$)	2.180	2.217	2.254				
C ($J K^{-1}mol^{-1}$)	441.0	448.4	455.9				



Name: Triphenylene
Formula: $C_{18}H_{12}$

CAS-RN: 217–59–4
Group No.: 14–080
Molar Mass: 228.29

TABLE 14.80.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71WON/WES	481.0–509.5	4	0.10	99.962	melpt	C_{sat}	BSAO	68WES/WES

TABLE 14.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	0.567	3.09–2	0.06	5.72–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
481.0–509.5		2.35548+2	–7.99810+1	8.76376			II

TABLE 14.80.4. Recommended values of heat capacities

Temp. (K)	480	490	500	510
c_{sat} (J K^{-1}g^{-1})	1.951	1.969	1.994	2.025
C_{sat} (J K^{-1}mol^{-1})	445.3	449.5	455.1	462.2

Name: 1,1':2',1''-Terphenyl
Formula: $C_{18}H_{14}$

CAS-RN: 84-15-1
Group No.: 14-081
Molar Mass: 230.31

TABLE 14.81.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72CHA/BES	330.1–355.6	14	0.10	99.995	melpt	C_p	BSAO	65STE/BLA

TABLE 14.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	14	14	0.489	2.33–2	0.05	2.02–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
330.1–355.6	2.03451+1	8.03673	II

TABLE 14.81.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_p (J K^{-1}g^{-1})	1.692	1.721	1.750
C_p (J K^{-1}mol^{-1})	389.7	396.4	403.0

Name: 1,1':3',1''-Terphenyl
Formula: $C_{18}H_{14}$

CAS-RN: 92-06-8
Group No.: 14-082
Molar Mass: 230.31

TABLE 14.82.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
58WAL/BRO	432.3–534.3	3	2.00	not specified		C_p	DSIO	56WAL/GRA

TABLE 14.82.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.017	1.97–2	0.03	–1.53–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
432.3–534.3	2.45197+1	6.93100	V

TABLE 14.82.4. Recommended values of heat capacities

Temp. (K)	440	450	460	470	480	490	500
c_p (J K^{-1}g^{-1})	1.99	2.01	2.04	2.06	2.09	2.11	2.14
C_p (J K^{-1}mol^{-1})	457	463	469	475	480	486	492
Temp. (K)	510	520	530				
c_p (J K^{-1}g^{-1})	2.16	2.19	2.21				
C_p (J K^{-1}mol^{-1})	498	504	509				

Name: 1,1':4',1''–Terphenyl
Formula: $C_{18}H_{14}$

CAS-RN: 92–94–4
Group No.: 14–083
Molar Mass: 230.31

TABLE 14.83.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83CHA	487.0–580.0	6S	0.50	99.9	chrom	C_p	BDHT	69PER/COM
93DUR/AOU	492.0–592.0	102	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 14.83.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83CHA	487.0–580.0	6	0.50	0.480	1.57–1	0.24	1.00–3	0
				Rejected data				
93DUR/AOU	(4.89, 8.35, –4.73, –90)							

TABLE 14.83.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	108	6	0.588	1.92–1	0.29	1.00–3	0
Temp. range K		A_1	A_2				Level of uncertainty
487.0–580.0		1.15041+1	9.63474				III

TABLE 14.83.4. Recommended values of heat capacities

Temp. (K)	490	500	510	520	530	540	550
c_p (J K^{-1}g^{-1})	2.120	2.154	2.189	2.224	2.259	2.294	2.328
C_p (J K^{-1}mol^{-1})	488.2	496.2	504.2	512.2	520.2	528.2	536.2
Temp. (K)	560	570	580				
c_p (J K^{-1}g^{-1})	2.363	2.398	2.433				
C_p (J K^{-1}mol^{-1})	544.3	552.3	560.3				

Name: 1–Methyl–7–(1–methylethyl)phenanthrene
Formula: $C_{18}H_{18}$

CAS-RN: 483–65–8
Group No.: 14–084
Molar Mass: 234.34

TABLE 14.84.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
44EIB	369.0–473.0	eqn	nosp	not specified	C_p	not specified	

TABLE 14.84.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	3.02–6	0.00	–3.82–7	0
Temp. range K		A_1	A_2				Level of uncertainty
369.0–473.4		2.16330+1	7.79479				V

TABLE 14.84.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p ($J\,K^{-1}g^{-1}$)	1.79	1.82	1.85	1.87	1.90	1.93	1.96
C_p ($J\,K^{-1}mol^{-1}$)	420	426	433	439	446	452	459
Temp. (K)	440	450	460	470			
c_p ($J\,K^{-1}g^{-1}$)	1.98	2.01	2.04	2.07			
C_p ($J\,K^{-1}mol^{-1}$)	465	472	478	484			

Name: *ar*,*ar'*–Bis(1–methylethyl)–1,1'–biphenyl
Formula: $C_{18}H_{22}$

CAS-RN: 36876–13–8
Group No.: 14–085
Molar Mass: 238.37

TABLE 14.85.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
56MCE/MAL	N	422.0–588.7	4S	nosp	not specified	C_p	not specified	

56MCE/MAL probably mixture of isomers

TABLE 14.85.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.034	4.68–2	0.07	–1.54–4	0
Temp. range K		A_1	A_2				Level of uncertainty
422.0–588.7		2.13374+1	9.78795				V

TABLE 14.85.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	2.18	2.21	2.25	2.28	2.31	2.35	2.38
C_p (J K^{-1}mol^{-1})	519	527	535	544	552	560	568
Temp. (K)	490	500	510	520	530	540	550
c_p (J K^{-1}g^{-1})	2.42	2.45	2.49	2.52	2.55	2.59	2.62
C_p (J K^{-1}mol^{-1})	576	584	592	601	609	617	625
Temp. (K)	560	570	580	590			
c_p (J K^{-1}g^{-1})	2.66	2.69	2.72	2.76			
C_p (J K^{-1}mol^{-1})	633	641	649	658			

Name: 1,1',1''–Methylidynetrisbenzene
Formula: $C_{19}H_{16}$

CAS-RN: 519–73–3
Group No.: 14–086
Molar Mass: 244.34

TABLE 14.86.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
17HIL/DUS	N	383.1	1	nosp	not specified	C_{avg}	DSIO	11LEW/RAN
32SPA/THO		373.1–383.1	2S	nosp	not specified	C_p	BDHO	31THO/PAR
44EIB		365.0–473.0	eqn	nosp	not specified	C_p	not specified	
50KUR		400.0–596.2	15	nosp	not specified	C_{avg}	DSIO	47KUR

17HIL/DUS average value in temperature range 369–408 K

TABLE 14.86.2. Correlated heat capacities

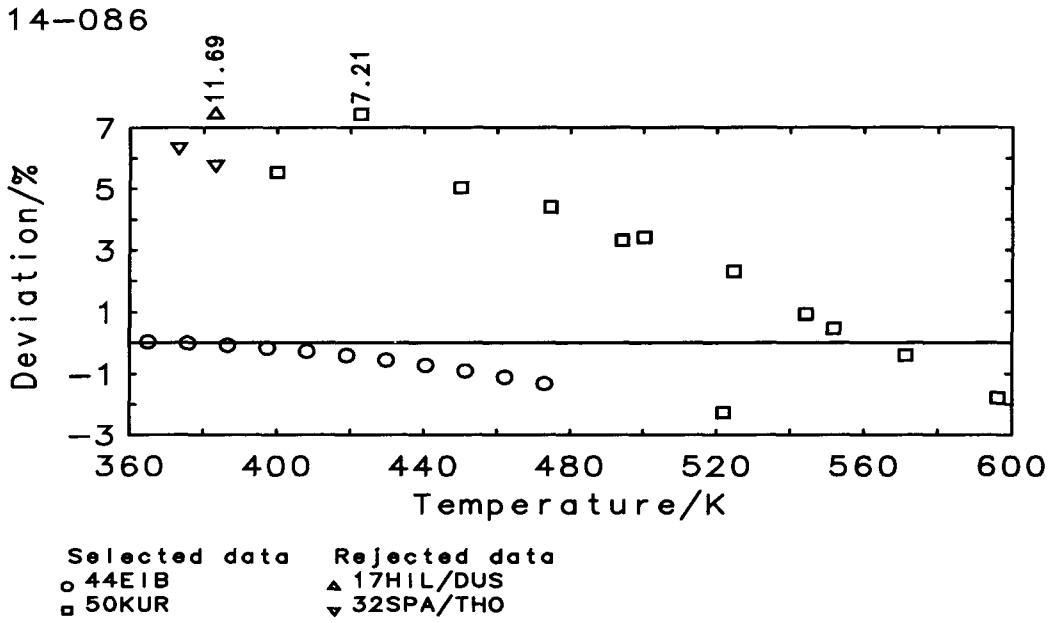
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
44EIB	365.0–465.0	11	1.00#	0.588	3.49–1	0.59	–2.57–1	–8
50KUR	400.0–596.2	15	3.00#	1.475	2.79	4.42	1.97	9
				Rejected data				
17HIL/DUS	(6.88, 11.69, 6.88, 1)		32SPA/THO	(3.33, 6.08, 3.33, 2)				

TABLE 14.86.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	26	1.259	2.27	3.60	1.02	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
365.0–596.2		1.76016+1	6.68562	5.98972–1			V

TABLE 14.86.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	1.72	1.76	1.80	1.84	1.87	1.91	1.95
C_p (J K^{-1}mol^{-1})	420	429	439	448	458	468	477
Temp. (K)	440	450	460	470	480	490	500
c_p (J K^{-1}g^{-1})	1.99	2.04	2.08	2.12	2.16	2.20	2.25
C_p (J K^{-1}mol^{-1})	487	497	507	518	528	538	549
Temp. (K)	510	520	530	540	550	560	570
c_p (J K^{-1}g^{-1})	2.29	2.33	2.38	2.42	2.47	2.51	2.56
C_p (J K^{-1}mol^{-1})	559	570	581	592	603	614	625
Temp. (K)	580	590	600				
c_p (J K^{-1}g^{-1})	2.60	2.65	2.70				
C_p (J K^{-1}mol^{-1})	636	648	659				



Name: Perylene
Formula: $C_{20}H_{12}$

CAS-RN: 198-55-0
Group No.: 14-087
Molar Mass: 252.32

TABLE 14.87.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80WON/WES	554.4–573.0	5	0.10	99.97	melpt	C_p	BSAO	68WES/WES
93DUR/AOU	552.0–652.0	51	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 14.87.2. Correlated heat capacities

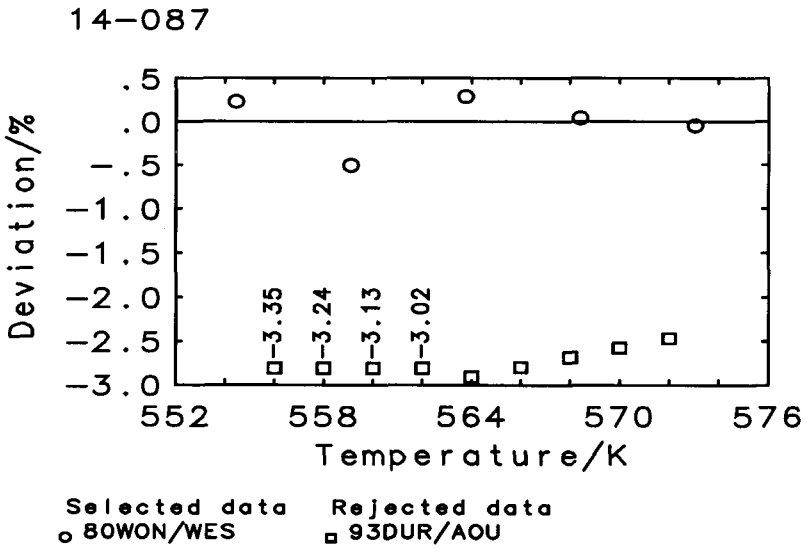
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
80WON/WES	554.4–573.0	5	0.30#	0.942	1.76–1	0.28	9.96–4	1
				Rejected data				
93DUR/AOU	(1.78, 2.92, –1.77, –9)							

TABLE 14.87.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	56	5	1.216	2.27–1	0.36	9.96–4	1
Temp. range K		A_1	A_2				Level of uncertainty
554.4–573.0		3.75800+1	4.44166				III

TABLE 14.87.4. Recommended values of heat capacities

Temp. (K)	560	570	580
c_p (J K^{-1}g^{-1})	2.058	2.073	2.087
C_p (J K^{-1}mol^{-1})	519.3	523.0	526.7



Name: 9,10–Dihydro–9,10[1',2']–benzenoanthracene
Formula: $C_{20}H_{14}$

CAS-RN: 477–75–8
Group No.: 14–088
Molar Mass: 254.33

TABLE 14.88.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70AND/WES	532.5–548.8	7	nosp	99.9995	melpt	C_p	BSAO	68WES/WES

TABLE 14.88.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.335	8.88–2	0.13	1.70–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
532.5–548.8		3.09320+1	6.56449				III

TABLE 14.88.4. Recommended values of heat capacities

Temp. (K)	530	540	550
c_p ($J K^{-1} g^{-1}$)	2.149	2.170	2.192
C_p ($J K^{-1} mol^{-1}$)	546.5	551.9	557.4

Name: 1–(2–Naphthalenylmethyl)naphthalene
Formula: $C_{21}H_{16}$

CAS-RN: 611–48–3
Group No.: 14–089
Molar Mass: 268.36

TABLE 14.89.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
77FIN/MES	343.3–422.9	10	0.20	99.9	melpt	C_{sat}	BSAO	47HUF

TABLE 14.89.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.207	2.34–2	0.04	1.33–5	–4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
343.3–422.9		9.86475	1.50534+1	–7.28695–1			II

TABLE 14.89.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	1.661	1.692	1.722	1.752	1.781	1.810	1.838
C_{sat} (J K^{-1}mol^{-1})	445.9	454.1	462.2	470.1	478.0	485.7	493.3
Temp. (K)	420						
c_{sat} (J K^{-1}g^{-1})	1.866						
C_{sat} (J K^{-1}mol^{-1})	500.8						

Name: Pentacene
Formula: $C_{22}H_{14}$

CAS-RN: 135–48–8
Group No.: 14–090
Molar Mass: 278.35

TABLE 14.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
93DUR/AOU	546.0–594.0	25	nosp	not specified		C_p	BDCT	86MER/BEN

TABLE 14.90.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	0.000	3.59–4	0.00	–9.15–7	0
Temp. range K		A_1	A_2				Level of uncertainty
546.0–594.0		1.05476+1	1.01792+1				VI

TABLE 14.90.4. Recommended values of heat capacities

Temp. (K)	550	560	570	580	590
c_p (J K^{-1}g^{-1})	1.99	2.02	2.05	2.08	2.11
C_p (J K^{-1}mol^{-1})	553	562	570	579	587

Name: 5'–Phenyl–1,1':3',1''–terphenyl
Formula: $C_{24}H_{18}$

CAS-RN: 612–71–5
Group No.: 14–091
Molar Mass: 306.41

TABLE 14.91.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82LEB/BYK	446.0–480.0	2S	2.00	99.4	melpt	C_p	BDHT	74DSM/COM

TABLE 14.91.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
446.0–480.0		1.49243+1	1.32652+1				V

TABLE 14.91.4. Recommended values of heat capacities

Temp. (K)	450	460	470	480
c_p (J K^{-1}g^{-1})	2.02	2.06	2.10	2.13
C_p (J K^{-1}mol^{-1})	620	631	642	653

Name: 1,1':3',1'':3'',1'''–Quaterphenyl
Formula: $C_{24}H_{18}$

CAS-RN: 1166–18–3
Group No.: 14–092
Molar Mass: 306.41

TABLE 14.92.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
58WAL/BRO	431.5–534.0	3	2.00	not specified		C_p	DSIO	56WAL/GRA

TABLE 14.92.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.009	1.40–2	0.02	1.27–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
431.5–534.0		3.48860+1	8.56650				V

TABLE 14.92.4. Recommended values of heat capacities

Temp. (K)	430	440	450	460	470	480	490
c_p (J K^{-1}g^{-1})	1.95	1.97	1.99	2.02	2.04	2.06	2.09
C_p (J K^{-1}mol^{-1})	596	603	611	618	625	632	639
Temp. (K)	500	510	520	530			
c_p (J K^{-1}g^{-1})	2.11	2.13	2.16	2.18			
C_p (J K^{-1}mol^{-1})	646	653	660	668			

Name: 1,1–Diphenyldodecane
Formula: $C_{24}H_{34}$

CAS-RN: 1603–53–8
Group No.: 14–093
Molar Mass: 322.53

TABLE 14.93.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60KAR/STR1	N	283.4–298.3	6	nosp	99.1	melpt	C_p	BSAO	54STR/ICK

60KAR/STR1 smoothed values in 60KAR/STR3

TABLE 14.93.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.373	2.64–1	0.37	1.31–3	0

Temp. range K	A_1	A_2	Level of uncertainty
283.4–298.3	4.90212+1	7.49856	IV

TABLE 14.93.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	1.824	1.840	1.844
C_p (J K^{-1}mol^{-1})	588.4	593.5	594.6

Name: (1–Cyclohexyldodecyl)benzene
Formula: $C_{24}H_{40}$

CAS-RN: 62155–50–4
Group No.: 14–094
Molar Mass: 328.58

TABLE 14.94.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60KAR/STR2	N	282.0–297.1	9	nosp	97.6	melpt	C_p	BSAO	54STR/ICK

60KAR/STR2 smoothed data in 60KAR/STR3

TABLE 14.94.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.178	1.30–1	0.18	3.64–4	1

Temp. range K	A_1	A_2	Level of uncertainty
282.0–297.1	5.65882+1	5.63261	IV

TABLE 14.94.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	1.845	1.857	1.860
C_p (J K^{-1}mol^{-1})	606.3	610.1	611.0

Name: 9,10–Diphenylanthracene
Formula: $C_{26}H_{18}$

CAS-RN: 1499–10–1
Group No.: 14–095
Molar Mass: 330.43

TABLE 14.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
93DUR/AOU	522.0–622.0	51	nosp	not specified	C_p	BDCT	86MER/BEN

TABLE 14.95.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	51	51	0.000	3.52–4	0.00	1.50–6	0
Temp. range K		A_1	A_2				Level of uncertainty
522.0–622.0		1.68489+1	1.19477+1				VI

TABLE 14.95.4. Recommended values of heat capacities

Temp. (K)	520	530	540	550	560	570	580
c_p ($J\,K^{-1}g^{-1}$)	1.99	2.02	2.05	2.08	2.11	2.14	2.17
C_p ($J\,K^{-1}mol^{-1}$)	657	667	677	686	696	706	716
Temp. (K)	590	600	610	620			
c_p ($J\,K^{-1}g^{-1}$)	2.20	2.23	2.26	2.29			
C_p ($J\,K^{-1}mol^{-1}$)	726	736	746	756			

Name: 11–Phenylheneicosane
Formula: $C_{27}H_{48}$

CAS-RN: 6703–80–6
Group No.: 14–096
Molar Mass: 372.68

TABLE 14.96.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
49PAR/MOO	300.00	2.054	nosp	not specified	C_p	BSIO	25PAR

Name: 1,1',1''–(1,3,5–Benzenetriyl)trisnaphthalene
Formula: $C_{36}H_{24}$

CAS-RN: 7059–70–3
Group No.: 14–097
Molar Mass: 456.59

TABLE 14.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
67MAG N	472.0–560.0	5	nosp	not specified	C_p	BDHT	66PER/COM

67MAG data from a graph only

TABLE 14.97.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.160	3.53–1	0.32	1.12–3	–3
Temp. range K		A_1	A_2				Level of uncertainty
472.0–560.0		4.07841+1	1.35793+1				V

TABLE 14.97.4. Recommended values of heat capacities

Temp. (K)	480	490	500	510	520	530	540
c_p ($J K^{-1} g^{-1}$)	1.93	1.95	1.98	2.00	2.03	2.05	2.08
C_p ($J K^{-1} mol^{-1}$)	881	892	904	915	926	937	949
Temp. (K)	550	560					
c_p ($J K^{-1} g^{-1}$)	2.10	2.13					
C_p ($J K^{-1} mol^{-1}$)	960	971					

2. Compounds of Carbon, Hydrogen and Halogen

21. Fluorine Drivatives

The fluorine derivatives family contains 33 compounds, three of which were measured at one temperature only.

Most measurements were carried out in the 1960's and 1970's at NPLT where data on 6 fluorinated benzenes and toluenes (65COU/GRI, 68COU/HAL1, 68COU/HAL2, 73AND/MAR1, 74AND/MAR) were obtained. The second laboratory which was involved in the study of these compounds, BMB (now called NIPER), performed measurements for four fluorinated benzenes and two fluorinated toluenes (56SCO/MCC1, 59SCO/DOU, 62SCO/MES, 63SCO/MES, 70MES/FIN). Data from both laboratories have uncertainties of 0.2 % and have been, therefore, included in the correlation. A similar situation holds for two data sets from NBSW (53FUR/MCC, 54FUR/MCC), two data sets from WRUC (67PAC/PLA, 69SMI/PAC), and one data set from UMMA (64TRO/WES2). On the other hand, the data contained in three articles originating from IICN (69PAU/LAV1, 71PAU, 75PAU1), have been rejected from the correlation because, in all cases, the data differed by 1 to 2 % from those of NPLT which we feel are more reliable. Exception has been made with the only available data for decafluorobiphenyl (71PAU/RAK).

Hexafluorobenzene has had its heat capacity measured most frequently. Accurate data (65COU/GRI, 70MES/FIN) have been supplemented by consistent data from IVTM (82GOR/SMI) with the reported error of 0.5 % for extending the upper temperature limit be several kelvins.

Low molar mass fluorinated alkanes and cycloalkanes are used as refrigerants and were thus measured repeatedly. Extensive measurements of temperature and pressure dependence far above the normal boiling temperature were carried out in the fSU (78SOL/SUK, 84STO/CHA) and data were published only as parameters of smoothing equations. In general, the data seem to have low accuracy. Also, for two substances, reliable low temperature data were available (measurements for trifluoromethane from UCB, 62VAL/BRO, and from CITP, 72COP/REA; measurements for octafluorocyclobutane from NBSW, 54FUR/MCC) which allowed one to extend the temperature range of recommendations considerably. Other Freons were measured at CIPT (44RUS/GOL, 72COP/REA) and at PSC (48PAC/AST).

Perfluorinated alkanes, C_5F_{12} and C_6F_{14}, were measured at the University of Strathclyde, Glasgow (74COC/NOR) using DSC and showed low accuracy over a limited temperature range. DSC measurements at UCCC (51OLI/GRI1) on C_7F_{16} were made and yielded results with high accuracy. Three differently hydrogenated and fluorinated naphthalenes were investigated at MSUM (81ZHO/KOS1) and results gave data having an estimated uncertainty of 0.5 %.

Name: Tetrafluoromethane
Formula: CF_4

CAS-RN: 75-73-0
Group No.: 21-001
Molar Mass: 88.00

TABLE 21.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38EUC/SCH	100.0–145.0	6S	nosp	99.9	estim	C_p	BSAO	38EUC/SCH
69ENO/SHI2	90.4–91.7	2	nosp	99.985	melpt	C_p	BSAO	66SHI/ATA
69SMI/PAC	92.0–139.9	21	nosp	99.985	melpt	C_{sat}	BSAO	55PAC/PIE
72COP/REA	121.6–141.4	6	nosp	99.9	estim	C_p	BSAO	68WES/FUR

TABLE 21.1.2. Correlated heat capacities

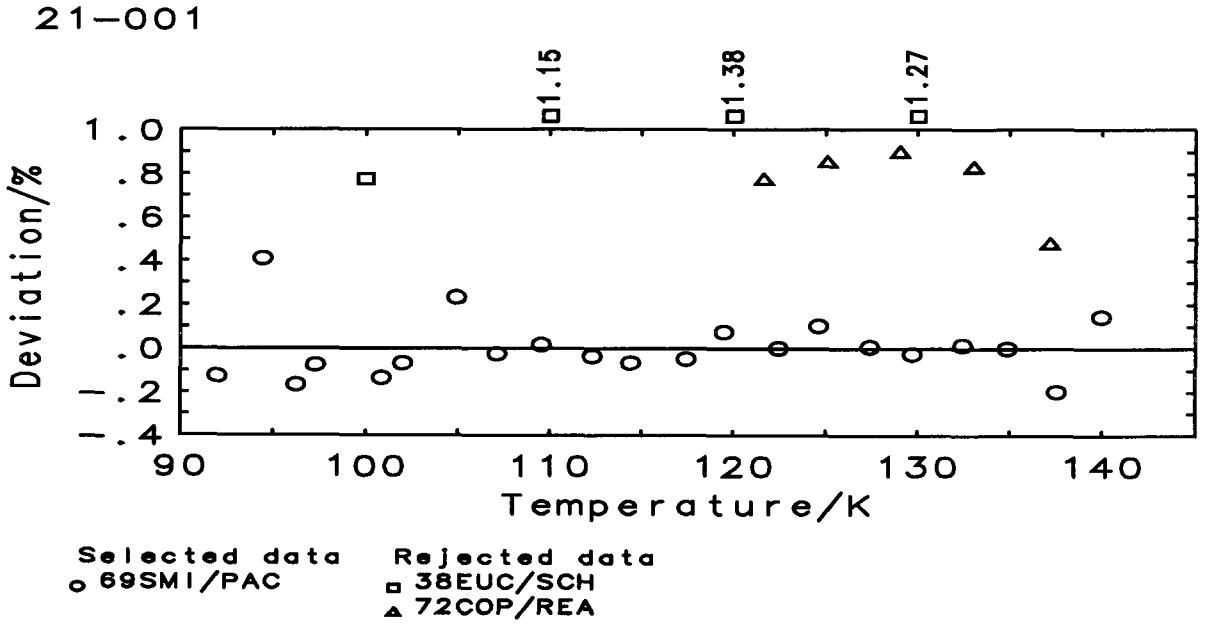
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
69SMI/PAC	92.0–139.9	21	0.20#	0.672	1.26–2	0.13	3.42–5	–4
				Rejected data				
38EUC/SCH	(1.10–1, 1.16, 1.08–1, 4)			72COP/REA	(7.32–2, 0.77, 7.18–2, 5)			

TABLE 21.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	35	21	0.725	1.36–2	0.15	3.42–5	–4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
92.0–139.9		1.28211+1	–6.39122	2.87755			II

TABLE 21.1.4. Recommended values of heat capacities

Temp. (K)	100	110	120	130	140
c_{sat} ($J K^{-1} g^{-1}$)	0.879	0.876	0.878	0.886	0.899
C_{sat} ($J K^{-1} mol^{-1}$)	77.39	77.10	77.29	77.95	79.10



Name: Trifluoromethane
Formula: CHF_3

CAS-RN: 75-46-7
Group No.: 21-002
Molar Mass: 70.01

TABLE 21.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62VAL/BRO	122.7–189.3	8	nosp	99.999	melpt	C_{sat}	BSIO	37GIA/EGA
72COP/REA	127.6–142.9	4	nosp	99.8	chrom	C_p	BSAO	68WES/FUR
78SOL/SUK	123.0–153.0	eqn	nosp	not specified		C_{sat}	BSAO	78SOL/SUK
78SOL/SUK	153.0–288.0	eqn	nosp	not specified		C_{sat}	BSAO	78SOL/SUK
84STO/CHA	173.0–191.0	eqn	0.30	99.98	anal	C_p	BSAO	78SOL/SUK

TABLE 21.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62VAL/BRO	122.7–189.3	8	0.30#	0.508	1.56–2	0.15	1.54–3	2
72COP/REA	127.6–142.9	4	0.20#	0.639	1.29–2	0.13	–5.40–3	–1
78SOL/SUK	123.0–153.0	5	1.00#	0.041	4.17–3	0.04	–1.49–4	1
78SOL/SUK	153.0–279.0	15	1.00#	0.594	8.57–2	0.59	–8.17–4	–5
84STO/CHA	173.0–191.0	5	0.30	0.266	8.20–3	0.08	8.02–3	5

TABLE 21.2.3. Parameters of cubic spline polynomials

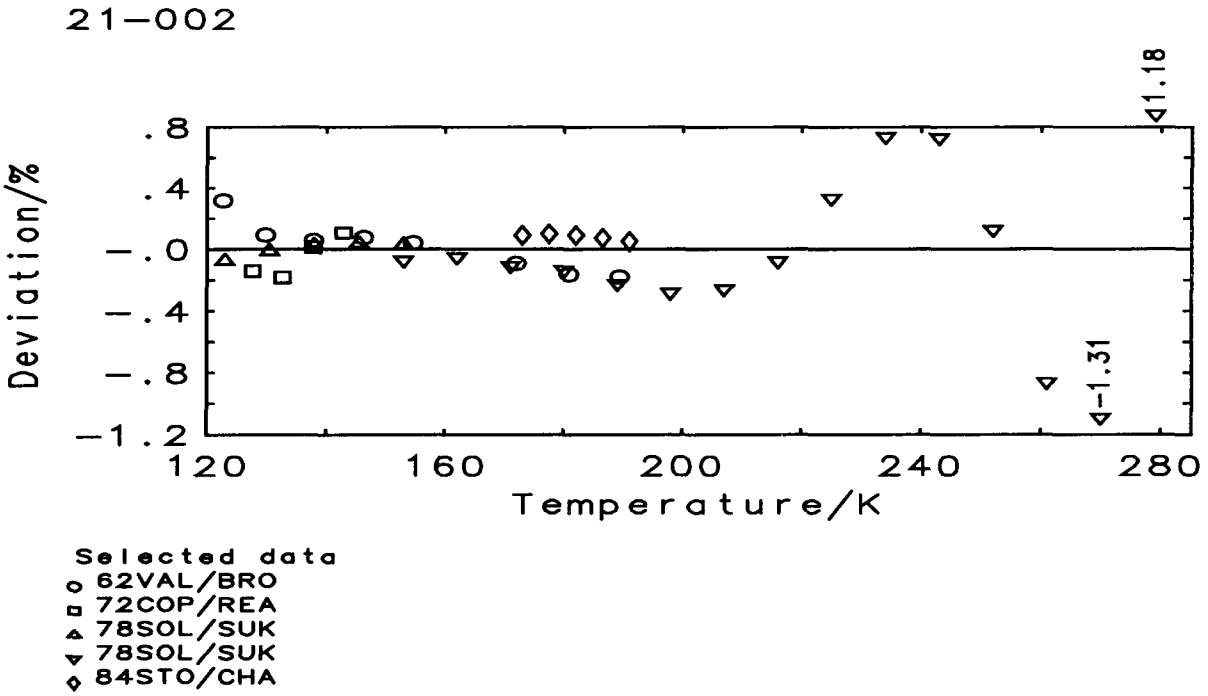
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	37	0.541	5.95–2	0.42	4.82–4	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
122.7–220.0		1.42801+1	–5.98233	2.25110	–9.23258–2		III
220.0–279.0		–1.75344+2	2.52596+2	–1.15284+2	1.77161+1		IV

TABLE 21.2.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_p ($J K^{-1} g^{-1}$)	1.209	1.200	1.195	1.195	1.199	1.207	1.219
C_p ($J K^{-1} mol^{-1}$)	84.67	84.01	83.67	83.64	83.92	84.49	85.36
Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1} g^{-1}$)	1.236	1.257	1.281	1.310	1.345	1.396	1.476
C_p ($J K^{-1} mol^{-1}$)	86.53	87.98	89.71	91.72	94.15	97.74	103.4
Temp. (K)	260	270	273.15	280			
c_p ($J K^{-1} g^{-1}$)	1.598	1.775	1.844	2.019			
C_p ($J K^{-1} mol^{-1}$)	111.9	124.3	129.1	141.3			

TABLE 21.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	37	0.966	4.20–2	0.40	9.71–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
122.7–279.0	299.30	–2.64123	2.72549–1	8.96704	3.34691	–1.67958+1	1.02816+1	IV



Name: Tetrafluoroethene
Formula: C_2F_4

CAS–RN: 116–14–3
Group No.: 21–003
Molar Mass: 100.02

TABLE 21.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53FUR/MCC	145.0–210.0	15S	0.20	99.99	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 21.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.070	1.80–3	0.01	8.27–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
145.0–210.0		1.49227+1	–3.63698	1.47869			II

TABLE 21.3.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} ($J K^{-1} g^{-1}$)	1.064	1.071	1.082	1.095	1.110	1.128	1.148
C_{sat} ($J K^{-1} mol^{-1}$)	106.4	107.2	108.2	109.5	111.0	112.8	114.8

TABLE 21.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	15	15	0.356	9.34-3	0.07	1.04-5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
145.0-210.0	306.50	5.98733-1	1.06879	1.10593+1	8.38519-2		II

Name: Hexafluoroethane
Formula: C_2F_6

CAS-RN: 76-16-4
Group No.: 21-004
Molar Mass: 138.01

TABLE 21.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48PAC/AST	174.9-190.7	10	0.50	99.84	melpt	C_p	BSIO	36AST/MES

TABLE 21.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.211	1.59-2	0.11	2.69-5	-1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
174.9-190.7		5.52188+1	-4.78117+1	1.41587+1			III

TABLE 21.4.4. Recommended values of heat capacities

Temp. (K)	180	185	190
c_p ($J K^{-1} g^{-1}$)	0.906	0.917	0.933
C_p ($J K^{-1} mol^{-1}$)	125.0	126.6	128.8

Name: 1,1,1–Trifluoroethane
Formula: $C_2H_3F_3$

CAS–RN: 420–46–2
Group No.: 21–005
Molar Mass: 84.04

TABLE 21.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
44RUS/GOL	165.4–220.7	11	0.10	99.95	melpt	C_p	BSAO	41YOS/GAR

TABLE 21.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.866	1.10–2	0.09	1.38–5	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
165.4–220.7		1.27400+1	–1.85308	9.34890–1			II

TABLE 21.5.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220
c_p ($J\,K^{-1}g^{-1}$)	1.216	1.230	1.246	1.264	1.283	1.305
C_p ($J\,K^{-1}mol^{-1}$)	102.2	103.4	104.7	106.2	107.9	109.7

TABLE 21.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.904	1.14–2	0.09	1.48–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
165.4–220.7	346.30	–8.09898–1	7.68275–1	1.01313+1	2.13444–1		II

Name: Octafluoropropane
Formula: C_3F_8

CAS–RN: 76–19–7
Group No.: 21–006
Molar Mass: 188.02

TABLE 21.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67PAC/PLA	125.8–233.0	36	0.10	99.993	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 21.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	36	36	0.983	6.71–2	0.34	4.63–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
125.8–233.0		1.28050+1	3.85835				III

TABLE 21.6.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J K^{-1}g^{-1})	0.788	0.805	0.822	0.839	0.856	0.873	0.890
C_{sat} (J K^{-1}mol^{-1})	148.2	151.4	154.6	157.8	161.0	164.2	167.4
Temp. (K)	200	210	220	230			
c_{sat} (J K^{-1}g^{-1})	0.907	0.925	0.942	0.959			
C_{sat} (J K^{-1}mol^{-1})	170.6	173.8	177.0	180.3			

TABLE 21.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	36	36	0.994	6.81–2	0.35	4.43–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
125.8–233.0	345.00	–2.84810–1	1.59589–3	1.29009+1	1.27071+1		III

Name: Octafluorocyclobutane
Formula: C_4F_8

CAS–RN: 115–25–3
Group No.: 21–007
Molar Mass: 200.03

TABLE 21.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
54FUR/MCC	234.7–268.5	9	0.20	99.98	melpt	C_{sat}	BSAO	45SCO/MEY
66VAS	237.1–316.9	17	0.80	99.8	melpt	C_{sat}	BDAO	64VAS2
84STO/CHA	233.0–267.0	eqn	0.30	99.98	anal	C_p	BSAO	78SOL/SUK

TABLE 21.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
54FUR/MCC	234.7–268.5	9	0.20	0.586	2.87–2	0.12	–1.27–2	–3
84STO/CHA	233.0–267.4	9	0.30	0.413	3.04–2	0.12	2.88–2	9
				Rejected data				
66VAS	(2.52, 11.44, –2.52, –9)							

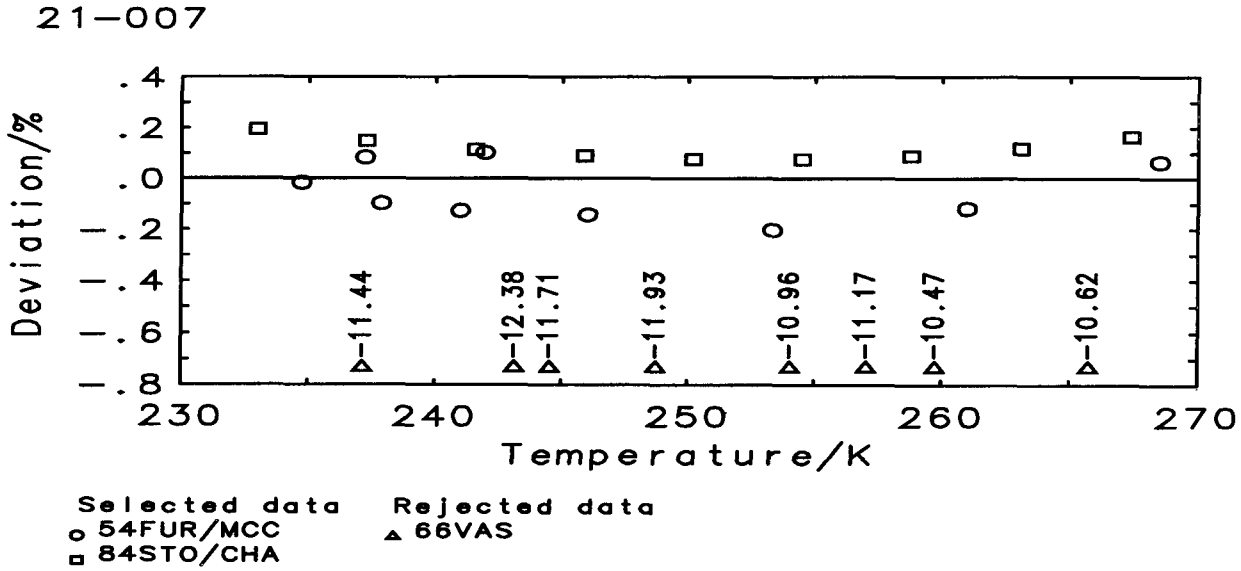
TABLE 21.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	35	18	0.538	3.14–2	0.13	8.07–3	6
C_{sat}	35	18	0.537	3.13–2	0.13	8.07–3	6

Temp. range K	A_1	A_2	Level of uncertainty
233.0–268.5	1.46654+1	3.95051	II
233.0–268.5	1.50684+1	3.77870	II

TABLE 21.7.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270
c_p (J K^{-1}g^{-1})	1.004	1.020	1.037	1.053
C_p (J K^{-1}mol^{-1})	200.8	204.1	207.3	210.6
c_{sat} (J K^{-1}g^{-1})	1.003	1.019	1.035	1.050
C_{sat} (J K^{-1}mol^{-1})	200.7	203.8	207.0	210.1



Name: Dodecafluoropentane
Formula: C_5F_{12}

CAS-RN: 678–26–2
Group No.: 21–008
Molar Mass: 288.04

TABLE 21.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74COC/NOR	N	233.0–253.0	3S	nosp	90.9	chrom	C_p	BDHT	69PER/COM

74COC/NOR impurity of 9.1 % due to branched perfluorohydrocarbons

TABLE 21.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.100	4.94–2	0.20	–5.72–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
233.0–253.0		–3.25881+1	2.34911+1				V

TABLE 21.8.4. Recommended values of heat capacities

Temp. (K)	230	240	250
c_p (J K^{-1}g^{-1})	0.62	0.69	0.75
C_p (J K^{-1}mol^{-1})	178	198	217

Name: 1,3–Difluoro–2,2–bis(fluoromethyl)propane
Formula: $C_5H_8F_4$

CAS–RN: 338–23–8
Group No.: 21–009
Molar Mass: 144.11

TABLE 21.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
64TRO/WES2	369.2–381.0	9	0.10	99.82	melpt	C_{sat}	BSAO	53WES/HAT

TABLE 21.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	1.712	5.23–2	0.17	–1.89–2	–5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
369.2–381.0		–1.05124+5	8.38439+4	–2.22836+4	1.97410+3		III

TABLE 21.9.4. Recommended values of heat capacities

Temp. (K)	370	375	380
c_{sat} (J K^{-1}g^{-1})	1.750	1.774	1.776
C_{sat} (J K^{-1}mol^{-1})	252.2	255.7	255.9

Name: Hexafluorobenzene
Formula: C_6F_6

CAS–RN: 392–56–3
Group No.: 21–010
Molar Mass: 186.06

TABLE 21.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65COU/GRE		281.9–305.9	8	0.20	99.97	melpt	C_p	BSAO	63AND/COU1
70MES/FIN		284.8–342.7	8	0.20	99.93	melpt	C_{sat}	BSAO	47HUF
82GOR/SIM	N	284.0–349.7	18	0.50	99.74	melpt	C_p	FSIO	83GOR/SIM
87WIL/LAI		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

82GOR/SIM same data in 82GOR/GRI

TABLE 21.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65COU/GRE	281.9–305.9	8	0.20	0.683	3.61–2	0.14	–8.53–3	–2
70MES/FIN	284.8–342.7	8	0.20	0.572	3.09–2	0.11	–3.49–3	0
82GOR/SIM	284.0–349.7	18	0.50	0.542	7.46–2	0.27	3.43–2	7
				Rejected data				
87WIL/LAI	(4.16–1, 1.54, 4.16–1, 1)							

TABLE 21.10.3. Parameters of regression polynomial

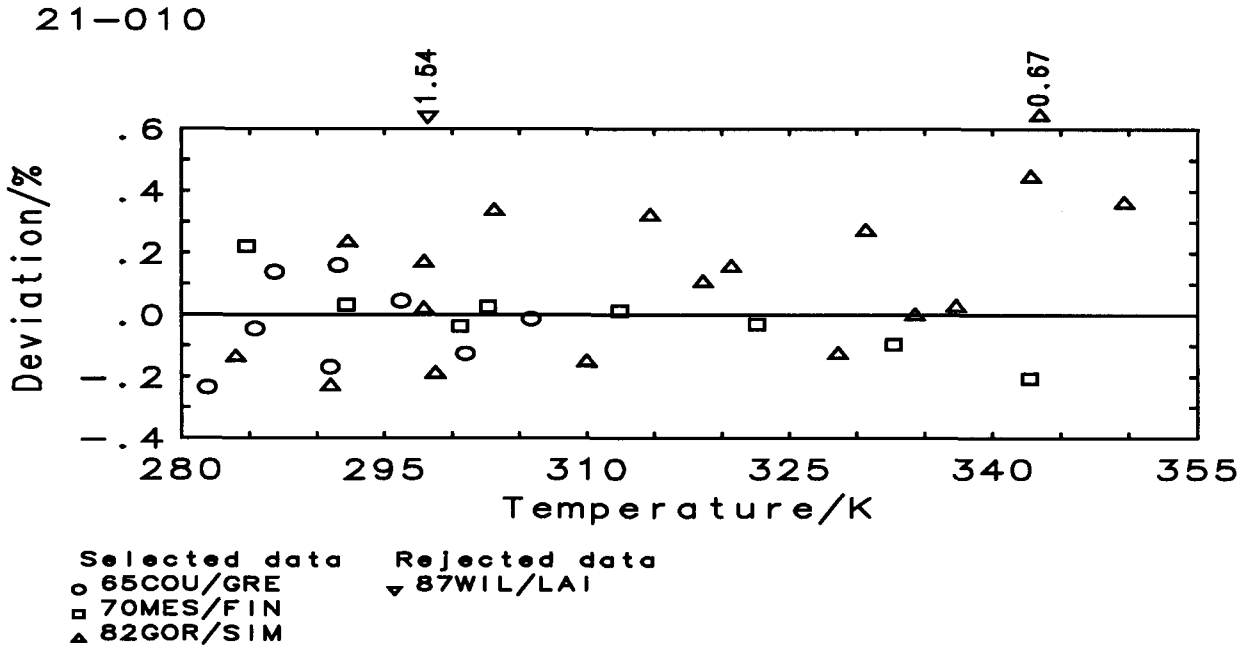
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	35	34	0.613	6.18–2	0.23	1.53–2	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
281.9–349.7		2.42710+1	–7.27364–1	5.11410–1			II

TABLE 21.10.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	1.173	1.183	1.191	1.193	1.203	1.215	1.226
C ($J K^{-1} mol^{-1}$)	218.2	220.0	221.6	221.9	223.9	226.0	228.1
Temp. (K)	340	350					
c ($J K^{-1} g^{-1}$)	1.238	1.251					
C ($J K^{-1} mol^{-1}$)	230.4	232.7					

TABLE 21.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	35	34	0.675	5.43–2	0.20	1.32–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
281.9–349.7	516.73	–2.56982	6.34040–1	2.14362+1	2.60393		II



Name: Tetradecafluorohexane
Formula: C_6F_{14}

CAS–RN: 355–42–0
Group No.: 21–011
Molar Mass: 338.04

TABLE 21.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74COC/NOR		233.0–273.0	5S	nosp	99.0	chrom	C_p	BDHT	69PER/COM
83CAM/DIA	N	293.0	1	nosp	not specified		C_p	BDHT	77LAG/PIE

83CAM/DIA a graph based on the same data in 82CAM/REY

TABLE 21.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74COC/NOR	233.0–273.0	5	3.00#	1.288	1.04	3.87	3.05–1	1
83CAM/DIA	293.0	1	3.00#	1.168	1.08	3.50	–1.08	–1

TABLE 21.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.554	1.28	4.66	7.50–2	0
Temp. range K		A_1	A_2				Level of uncertainty
233.0–293.0		–1.92412+1	1.74106+1				VI

TABLE 21.11.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	0.51	0.55	0.60	0.64	0.68	0.70	0.73
C_p ($J K^{-1}mol^{-1}$)	173	187	202	216	231	235	245
Temp. (K)	290	298.15	300				
c_p ($J K^{-1}g^{-1}$)	0.77	0.80	0.81				
C_p ($J K^{-1}mol^{-1}$)	260	272	274				

Name: Pentafluorobenzene
Formula: C_6HF_5

CAS-RN: 363-72-4
Group No.: 21-012
Molar Mass: 168.07

TABLE 21.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
68COU/HAL2	230.7–324.1	21	nosp	99.87	melpt	C_p	BSAO	63AND/COU1
69PAU/LAV1	230.3–300.4	11	nosp	99.46	melpt	C_{sat}	BSAO	69PAU/LAV2

TABLE 21.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68COU/HAL2	230.7–324.1	21	0.20#	0.241	1.17–2	0.05	1.18–5	2
				Rejected data				
69PAU/LAV1	(5.22–1, 2.13, 5.07–1, 10)							

TABLE 21.12.3. Parameters of regression polynomial

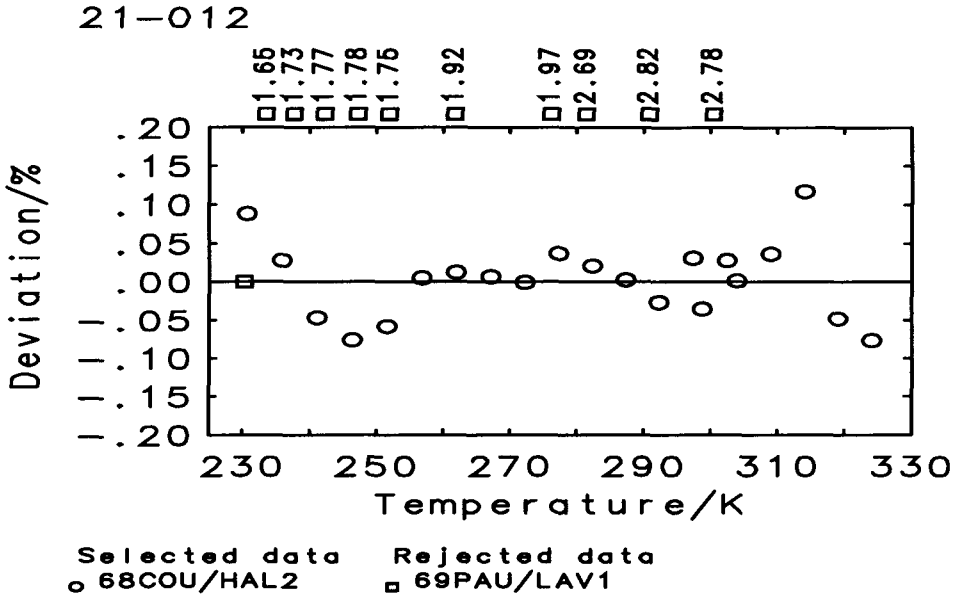
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	21	0.260	1.26–2	0.05	1.18–5	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
230.7–324.1		1.95493+1	5.61347–1	3.82448–1			II

TABLE 21.12.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.131	1.143	1.155	1.167	1.180	1.184	1.193
C_p ($J K^{-1}mol^{-1}$)	190.1	192.1	194.1	196.2	198.3	199.0	200.5
Temp. (K)	290	298.15	300	310	320	330	
c_p ($J K^{-1}g^{-1}$)	1.207	1.218	1.221	1.235	1.250	1.265	
C_p ($J K^{-1}mol^{-1}$)	202.8	204.7	205.2	207.6	210.0	212.6	

TABLE 21.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	21	0.288	1.39–2	0.06	1.46–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
230.7–324.1	532.00	–3.07933	3.92423–1	1.78115+1	6.04087		II



Name: 1,2,3,4–Tetrafluorobenzene
Formula: $C_6H_2F_4$

CAS–RN: 551–62–2
Group No.: 21–013
Molar Mass: 150.08

TABLE 21.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73AND/MAR1	235.5–319.8	41	nosp	99.85	melpt	C_p	BSAO	63AND/COU1

TABLE 21.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	41	0.296	1.30–2	0.06	1.37–5	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
235.5–319.8		–2.62887	2.14433+1	–6.81722	8.35405–1		II

TABLE 21.13.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.170	1.187	1.203	1.220	1.225	1.236	1.252
C_p (J K^{-1}mol^{-1})	175.6	178.1	180.6	183.0	183.8	185.4	187.9
Temp. (K)	298.15	300	310	320			
c_p (J K^{-1}g^{-1})	1.266	1.269	1.286	1.305			
C_p (J K^{-1}mol^{-1})	189.9	190.4	193.1	195.9			

TABLE 21.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	41	0.371	1.66–2	0.07	2.23–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
235.5–319.8	550.80	–1.46170	3.98380–2	1.43733+1	1.34079+1		II

Name: 1,2,3,5–Tetrafluorobenzene
Formula: $C_6H_2F_4$

CAS–RN: 2367–82–0
Group No.: 21–014
Molar Mass: 150.08

TABLE 21.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73AND/MAR1	229.3–311.2	25	nosp	99.99	melpt	C_p	BSAO	63AND/COU1

TABLE 21.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	0.335	1.49–2	0.07	1.89–5	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
229.3–311.2		1.94897+1	–1.02669	7.26879–1			II

TABLE 21.14.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.162	1.175	1.189	1.204	1.220	1.225	1.236
C_p (J K^{-1}mol^{-1})	174.4	176.4	178.5	180.7	183.1	183.8	185.5
Temp. (K)	290	298.15	300	310			
c_p (J K^{-1}g^{-1})	1.253	1.268	1.272	1.290			
C_p (J K^{-1}mol^{-1})	188.1	190.3	190.8	193.7			

TABLE 21.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	25	25	0.309	1.37–2	0.06	1.49–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
229.3–311.2	535.20	–3.38317	1.68047	1.53904+1	1.70277		II

Name: 1,2,4,5–Tetrafluorobenzene
Formula: $C_6H_2F_4$

CAS–RN: 327–54–8
Group No.: 21–015
Molar Mass: 150.08

TABLE 21.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73AND/MAR1	279.8–352.5	20	nosp	99.94	melpt	C_p	BSAO	63AND/COU1

TABLE 21.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	20	20	0.284	1.33–2	0.06	1.27–5	1
Temp. range K		A_1	A_2				Level of uncertainty
279.8–352.5		1.41727+1	3.00019				II

TABLE 21.15.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.251	1.267	1.281	1.284	1.300	1.317	1.334
C_p ($J\,K^{-1}mol^{-1}$)	187.7	190.2	192.2	192.7	195.2	197.7	200.2
Temp. (K)	340	350					
c_p ($J\,K^{-1}g^{-1}$)	1.350	1.367					
C_p ($J\,K^{-1}mol^{-1}$)	202.7	205.1					

TABLE 21.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	20	20	0.292	1.37–2	0.06	1.31–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
279.8–352.5	543.30	1.36161–1	2.78781–4	1.41018+1	1.66257+1		II

Name: 1,2–Difluorobenzene
Formula: $C_6H_4F_2$

CAS–RN: 367–11–3
Group No.: 21–016
Molar Mass: 114.09

TABLE 21.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63SCO/MES	229.0–357.2	20	0.20	99.998	melpt	C_{sat}	BSAO	47HUF

TABLE 21.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.252	1.02–2	0.05	8.01–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
229.0–357.2		2.32770+1	–1.04138+1	4.52483	–5.02627–1		II

TABLE 21.16.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.250	1.268	1.288	1.308	1.330	1.337	1.352
C_{sat} (J K^{-1}mol^{-1})	142.6	144.7	146.9	149.3	151.8	152.6	154.3
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.375	1.394	1.398	1.421	1.444	1.467	1.488
C_{sat} (J K^{-1}mol^{-1})	156.9	159.1	159.5	162.2	164.8	167.3	169.8
Temp. (K)	350	360					
c_{sat} (J K^{-1}g^{-1})	1.509	1.529					
C_{sat} (J K^{-1}mol^{-1})	172.2	174.4					

TABLE 21.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.735	2.85–2	0.15	7.70–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
229.0–357.2	562.50	–1.11457	2.14668–2	1.05712+1	1.44674+1		II

Name: 1,3–Difluorobenzene
Formula: $C_6H_4F_2$

CAS–RN: 372–18–9
Group No.: 21–017
Molar Mass: 114.09

TABLE 21.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70MES/FIN	214.3–354.9	15	0.20	99.999	melpt	C_{sat}	BSAO	47HUF

TABLE 21.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.090	3.16–3	0.02	1.91–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
214.3–354.9		1.84883+1	–5.05609	2.51870	–2.51541–1		II

TABLE 21.17.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.213	1.230	1.248	1.267	1.287	1.308	1.330
C_{sat} (J K^{-1}mol^{-1})	138.4	140.3	142.4	144.5	146.8	149.2	151.7
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.337	1.352	1.375	1.395	1.399	1.423	1.447
C_{sat} (J K^{-1}mol^{-1})	152.5	154.3	156.9	159.1	159.6	162.3	165.1
Temp. (K)	330	340	350	360			
c_{sat} (J K^{-1}g^{-1})	1.471	1.496	1.520	1.544			
C_{sat} (J K^{-1}mol^{-1})	167.9	170.7	173.5	176.2			

TABLE 21.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.716	2.67–2	0.14	6.50–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
214.3–354.9	543.00	–3.37293	3.64435–1	1.13396+1	7.80431		II

Name: 1,4–Difluorobenzene
Formula: $C_6H_4F_2$

CAS–RN: 540–36–3
Group No.: 21–018
Molar Mass: 114.09

TABLE 21.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91LIC	N	238.0–324.0	eqn	2.00	99.	anal	C_p	BDCT	89BRE/LIC

91LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 21.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
238.0–324.4		1.34746+1	1.90029				V

TABLE 21.18.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	1.31	1.33	1.34	1.36	1.36	1.37	1.38
C_p ($J K^{-1}mol^{-1}$)	150	152	153	155	155	156	158
Temp. (K)	298.15	300	310	320			
c_p ($J K^{-1}g^{-1}$)	1.39	1.40	1.41	1.43			
C_p ($J K^{-1}mol^{-1}$)	159	159	161	163			

Name: Fluorobenzene
Formula: C_6H_5F

CAS–RN: 462–06–6
Group No.: 21–019
Molar Mass: 96.10

TABLE 21.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37STU	240.0–320.0	9S	nosp	not specified		C_p	BDHO	37STU
56SCO/MCC1	235.1–350.3	16	0.10	99.97	melpt	C_{sat}	BSAO	43RUE/HUF
84ROU/GRO	298.1	1	0.30	99.	estim	C_p	FSIT	71PIC/LED

TABLE 21.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56SCO/MCC1	235.1–350.3	16	0.10	0.174	2.94–3	0.02	3.02–5	1
84ROU/GRO	298.1	1	0.30	0.080	4.20–3	0.02	–4.20–3	–1
				Rejected data				
37STU	(3.67–1, 2.15, 2.28–1, 3)							

TABLE 21.19.3. Parameters of regression polynomial

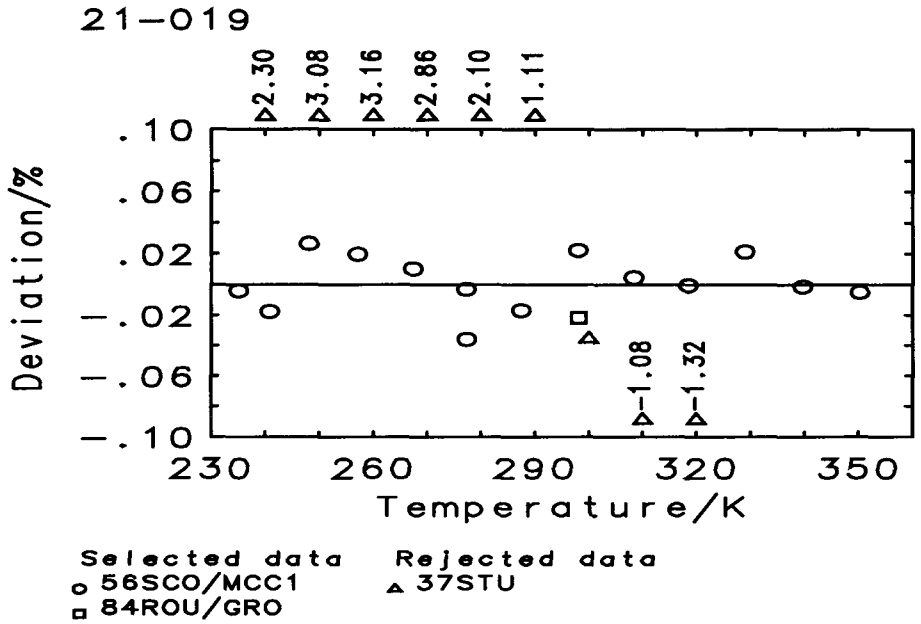
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	26	17	0.194	3.46–3	0.02	–2.19–4	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
235.1–350.3		2.02402+1	–7.30473	3.00091	–2.84436–1		II

TABLE 21.19.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1}g^{-1}$)	1.390	1.409	1.431	1.453	1.460	1.477	1.502
C ($J K^{-1}mol^{-1}$)	133.5	135.4	137.5	139.6	140.4	141.9	144.3
Temp. (K)	298.15	300	310	320	330	340	350
c ($J K^{-1}g^{-1}$)	1.523	1.527	1.554	1.581	1.609	1.636	1.665
C ($J K^{-1}mol^{-1}$)	146.3	146.8	149.3	151.9	154.6	157.3	160.0

TABLE 21.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	26	17	1.047	1.93–2	0.10	–2.82–3	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
235.1–350.3	560.09	–3.82528	9.64460–1	1.06013+1	3.79301		II



Name: Pentafluoro(trifluoromethyl)benzene
Formula: C_7F_8

CAS-RN: 434–64–0
Group No.: 21–020
Molar Mass: 236.06

TABLE 21.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74AND/MAR	210.8–365.1	36	nosp	99.89	melpt	C_p	BSAO	63AND/COU1
75PAU1	210.8–298.8	23	nosp	99.47	melpt	C_{sat}	BSAO	69PAU/LAV2

TABLE 21.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74AND/MAR	210.8–365.1	36	0.20#	0.193	1.19–2	0.04	7.79–6	–1
				Rejected data				
75PAU1	(4.12–1, 1.34, 4.04–1, 22)							

TABLE 21.20.3. Parameters of regression polynomial

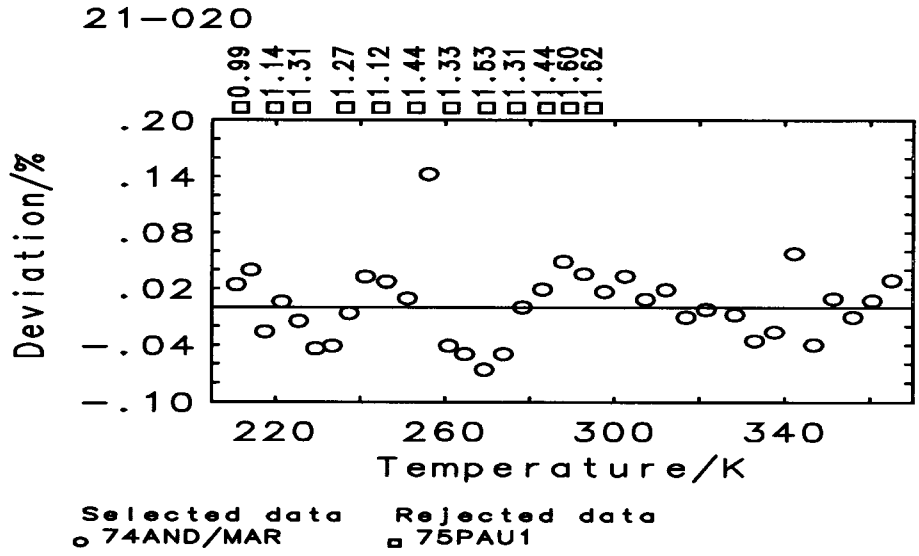
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	59	36	0.205	1.26–2	0.04	7.79–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
210.8–365.1		3.12549+1	–5.68404	2.70101	–2.55401–1		II

TABLE 21.20.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.017	1.025	1.034	1.044	1.054	1.065	1.077
C_p (J K^{-1}mol^{-1})	240.0	242.0	244.1	246.4	248.9	251.5	254.2
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.080	1.089	1.101	1.111	1.114	1.126	1.140
C_p (J K^{-1}mol^{-1})	255.1	257.0	259.9	262.3	262.9	265.9	269.0
Temp. (K)	330	340	350	360	370		
c_p (J K^{-1}g^{-1})	1.153	1.166	1.180	1.193	1.207		
C_p (J K^{-1}mol^{-1})	272.2	275.3	278.5	281.7	284.9		

TABLE 21.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	59	36	0.565	3.49–2	0.11	7.40–5	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
210.8–365.1	534.47	–3.70808	4.36801–1	2.31329+1	7.86963		II



Name: (Trifluoromethyl)undecafluorocyclohexane
Formula: C_7F_{14}

CAS-RN: 355-02-2
Group No.: 21-021
Molar Mass: 350.05

TABLE 21.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57YAR/KAY	303.0–335.0	eqn	1.10	not specified		C_p	BSIO	75PED/KAY

TABLE 21.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.000	2.95–6	0.00	1.63–6	0
Temp. range K		A_1	A_2				Level of uncertainty
303.0–334.8		2.35457+1	6.34151				V

TABLE 21.21.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	1.01	1.03	1.04	1.06	1.07
C_p ($J\,K^{-1}mol^{-1}$)	354	359	364	370	375

Name: Hexadecafluoroheptane
Formula: C_7F_{16}

CAS-RN: 335-57-9
Group No.: 21-022
Molar Mass: 388.05

TABLE 21.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51OLI/GRI1	221.9–310.0	10S	0.20	99.94	melpt	C_{sat}	BSAO	43RUE/HUF
57YAR/KAY	295.0–345.0	eqn	1.10	not specified		C_p	BSIO	75PED/KAY

TABLE 21.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
51OLI/GRI1	221.9–310.0	10	0.20	0.154	1.43–2	0.03	–4.96–6	–1
			Rejected data					
57YAR/KAY	(8.55–1, 1.72, –8.53–1, –3)							

TABLE 21.22.3. Parameters of regression polynomial

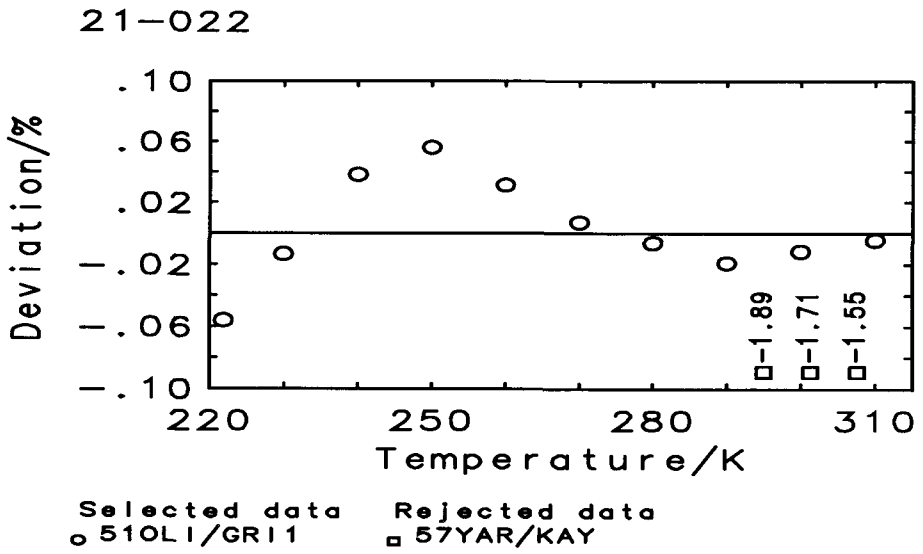
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	10	0.172	1.60–2	0.03	–4.96–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
221.9–310.0		3.01875+1	6.75732				II

TABLE 21.22.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	0.965	0.980	0.994	1.009	1.023	1.038	1.042
C_{sat} (J K^{-1}mol^{-1})	374.6	380.2	385.8	391.5	397.1	402.7	404.5
Temp. (K)	280	290	298.15	300	310		
c_{sat} (J K^{-1}g^{-1})	1.052	1.067	1.078	1.081	1.096		
C_{sat} (J K^{-1}mol^{-1})	408.3	413.9	418.5	419.5	425.2		

TABLE 21.22.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	10	0.146	1.39–2	0.03	3.82–6	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
221.9–310.0	474.80	1.14138	9.40148–3	2.96808+1	3.46421+1		II



Name: Pentafluoromethylbenzene
Formula: $C_7H_3F_5$

CAS-RN: 771-56-2
Group No.: 21-023
Molar Mass: 182.09

TABLE 21.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
68COU/HAL1		252.8–376.5	30	nosp	99.95	melpt	C_p	BSAO	63AND/COU1
71PAU2	N	243.7–305.0	9S	nosp	not specified		C_{sat}	BSAO	69PAU/LAV2

71PAU2 measured data deposited in VINITI No 2538-71

TABLE 21.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68COU/HAL1	252.8–376.5	30	0.20#	0.222	1.23–2	0.04	1.20–5	1
				Rejected data				
71PAU2	(5.51–1, 2.01, 5.45–1, 7)							

TABLE 21.23.3. Parameters of regression polynomial

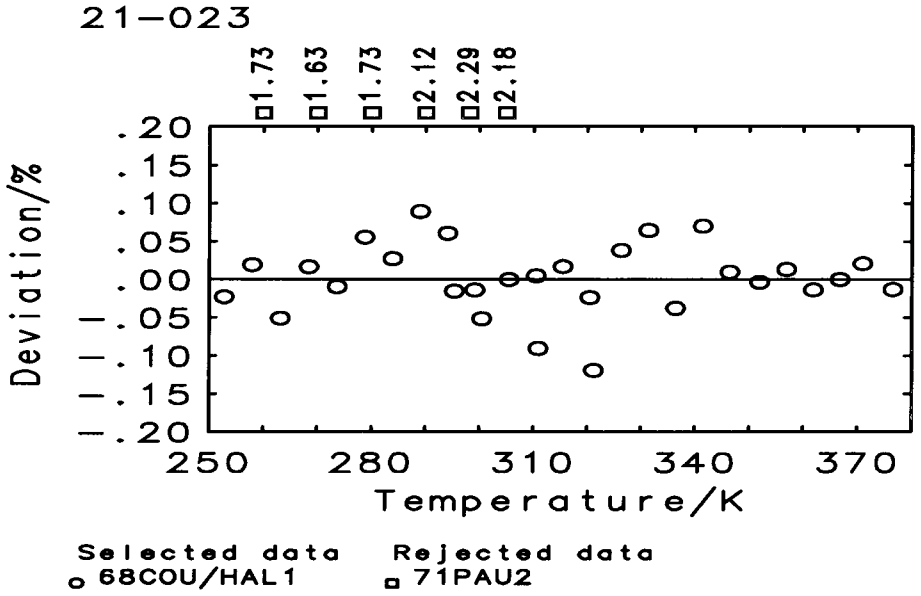
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	30	0.234	1.29–2	0.05	1.20–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
252.8–376.5		1.89055+1	2.03596	2.46068–1			II

TABLE 21.23.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.166	1.181	1.196	1.201	1.212	1.227	1.240
C_p (J K^{-1}mol^{-1})	212.3	215.0	217.8	218.7	220.6	223.5	225.8
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.243	1.259	1.276	1.292	1.309	1.326	1.344
C_p (J K^{-1}mol^{-1})	226.4	229.3	232.3	235.3	238.4	241.5	244.6
Temp. (K)	370	380					
c_p (J K^{-1}g^{-1})	1.361	1.379					
C_p (J K^{-1}mol^{-1})	247.8	251.1					

TABLE 21.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	30	0.236	1.31–2	0.05	1.04–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
252.8–376.5	566.50	–2.52279	1.14009–1	1.76947+1	1.39561+1		II



Name: (Trifluoromethyl)benzene
Formula: $C_7H_5F_3$

CAS–RN: 98–08–8
Group No.: 21–024
Molar Mass: 146.11

TABLE 21.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59SCO/DOU	252.5–364.7	13	0.20	99.9987	melpt	C_{sat}	BSAO	47HUF
89JAD/FRA	325.0–365.0	5	nosp	99.	anal	C_p	BDCT	86MER/BEN

TABLE 21.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59SCO/DOU	252.5–364.7	13	0.20	0.153	6.94–3	0.03	4.26–6	3
				Rejected data				
89JAD/FRA	(5.37–1, 2.09, 4.29–1, 4)							

TABLE 21.24.3. Parameters of regression polynomial

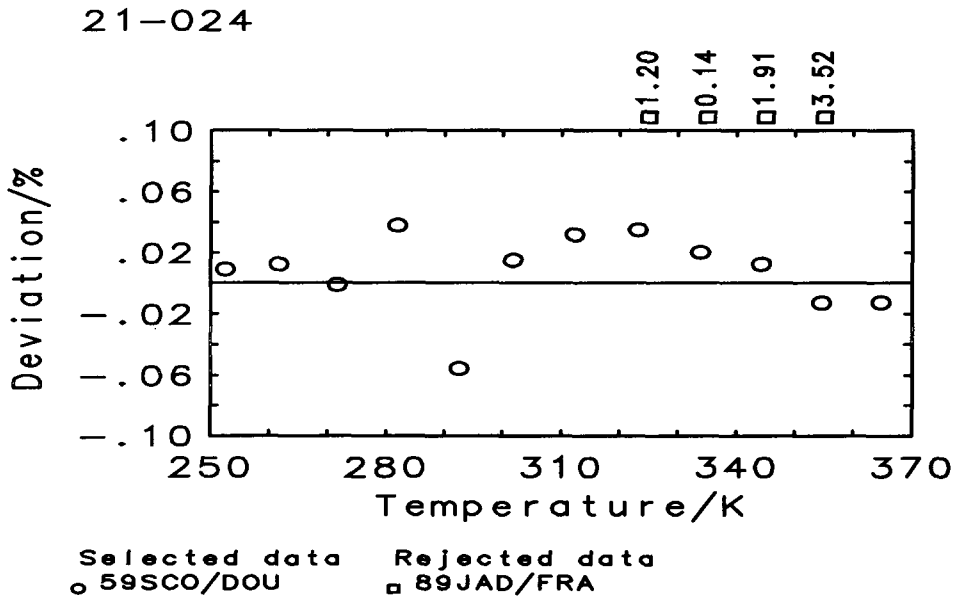
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	13	0.174	7.91–3	0.03	4.26–6	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
252.5–364.7		1.30944+1	2.32085	2.98263–1			II

TABLE 21.24.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.181	1.203	1.225	1.233	1.248	1.271	1.290
C_{sat} (J K^{-1}mol^{-1})	172.6	175.8	179.1	180.1	182.3	185.7	188.5
Temp. (K)	300	310	320	330	340	350	360
c_{sat} (J K^{-1}g^{-1})	1.294	1.318	1.342	1.366	1.390	1.415	1.441
C_{sat} (J K^{-1}mol^{-1})	189.1	192.5	196.0	199.6	203.1	206.8	210.5
Temp. (K)	370						
c_{sat} (J K^{-1}g^{-1})	1.466						
C_{sat} (J K^{-1}mol^{-1})	214.2						

TABLE 21.24.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	13	0.213	9.78–3	0.04	6.31–6	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
252.5–364.7	562.60	–3.07158	1.49560–1	1.16726+1	1.57706+1		II



Name: 1–Fluoro–2–methylbenzene
Formula: C_7H_7F

CAS–RN: 95–52–3
Group No.: 21–025
Molar Mass: 110.13

TABLE 21.25.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90MEV/LIC	210.65	1.298	3.00	99.	anal	C_p	BDCT	89BRE/LIC

Name: 1–Fluoro–3–methylbenzene
Formula: C_7H_7F

CAS–RN: 352–70–5
Group No.: 21–026
Molar Mass: 110.13

TABLE 21.26.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90MEV/LIC	183.95	1.217	3.00	99.	anal	C_p	BDCT	89BRE/LIC

Name: 1–Fluoro–4–methylbenzene
Formula: C_7H_7F

CAS–RN: 352–32–9
Group No.: 21–027
Molar Mass: 110.13

TABLE 21.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62SCO/MES		221.4–360.5	19	0.20	99.92	melpt	C_{sat}	BSAO	47HUF
90MEV/LIC	N	216.0–298.0	eqn	3.00	99.	anal	C_p	BDCT	89BRE/LIC

90MEV/LIC same equation in 91LIC

TABLE 21.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62SCO/MES	221.4–360.5	19	0.20	0.171	7.35–3	0.03	1.81–6	–2
				Rejected data				
90MEV/LIC	(2.25–1, 1.14, 5.15–2, 0)							

TABLE 21.27.3. Parameters of regression polynomial

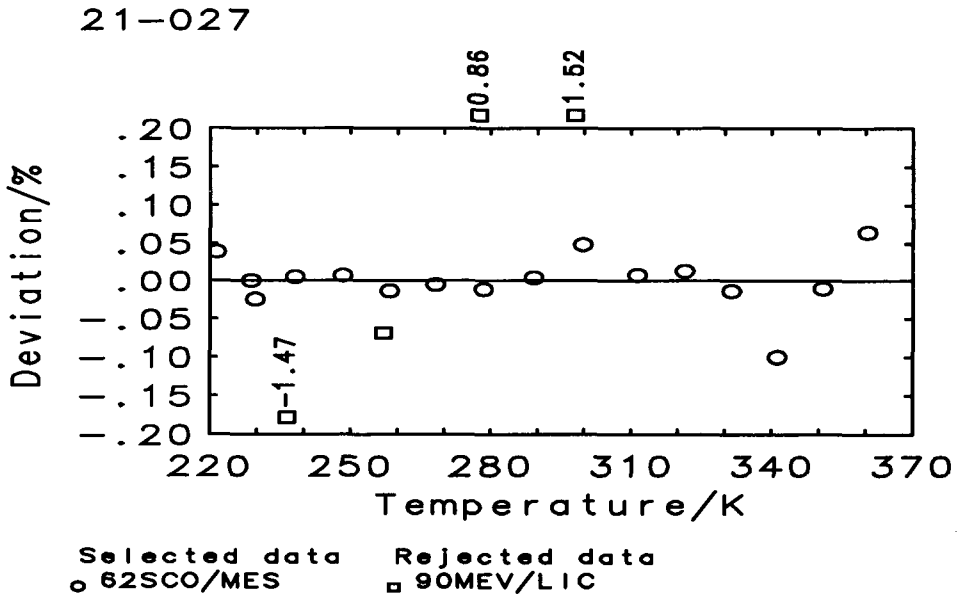
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	19	0.192	8.27–3	0.04	1.81–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
221.4–360.5		2.54744+1	–1.15407+1	4.89196	–5.27311–1		II

TABLE 21.27.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	1.370	1.389	1.409	1.431	1.455	1.480	1.488
C_{sat} (J K^{-1}mol^{-1})	150.9	152.9	155.2	157.6	160.2	162.9	163.8
Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.505	1.532	1.553	1.558	1.585	1.613	1.639
C_{sat} (J K^{-1}mol^{-1})	165.8	168.7	171.1	171.6	174.6	177.6	180.5
Temp. (K)	340	350	360				
c_{sat} (J K^{-1}g^{-1})	1.666	1.691	1.716				
C_{sat} (J K^{-1}mol^{-1})	183.4	186.2	189.0				

TABLE 21.27.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	19	0.959	3.81–2	0.19	1.28–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
221.4–360.5	589.20	–3.80900	3.34663–1	1.17122+1	1.08381+1		II



Name: Decafluorobis(trifluoromethyl)cyclohexane
Formula: C_8F_{16}

CAS-RN: 26637-68-3
Group No.: 21-028
Molar Mass: 400.06

TABLE 21.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
57YAR/KAY	N	304.0–360.0	eqn	1.10	not specified		C_p	BSIO	75PED/KAY

57YAR/KAY probably mixture of isomers (according to n.b.t.)

TABLE 21.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.000	1.91–6	0.00	6.36–7	0

Temp. range K	A_1	A_2	Level of uncertainty
304.0–360.0	2.95116+1	6.44217	V

TABLE 21.28.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1}g^{-1}$)	1.02	1.03	1.04	1.06	1.07	1.08	1.10
C_p ($J K^{-1}mol^{-1}$)	406	411	417	422	427	433	438

Temp. (K)	370
c_p ($J K^{-1}g^{-1}$)	1.11
C_p ($J K^{-1}mol^{-1}$)	444

Name: Octadecafluorooctane
Formula: C_8F_{18}

CAS-RN: 307-34-6
Group No.: 21-029
Molar Mass: 438.06

TABLE 21.29.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83CAM/DIA	N	293.00	0.8883	nosp	not specified		C_p	BDHT	77LAG/PIE

83CAM/DIA a graph based on the same data in 82CAM/REY

Name: Hexadecafluoro-1,2,3,4,5,6,7,8-octahydronaphthalene
Formula: $C_{10}F_{16}$

CAS-RN: 54939-04-7
Group No.: 21-030
Molar Mass: 424.08

TABLE 21.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81ZHO/KOS2	266.8–300.8	7	nosp	99.59	melpt	C_{sat}	BSAO	79ZHO/KOS

TABLE 21.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.136	3.41–2	0.07	3.76–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
266.8–300.8		2.64594+1	8.42922				IV

TABLE 21.30.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	0.965	0.970	0.981	0.998	1.011	1.015
C_{sat} (J K^{-1}mol^{-1})	409.2	411.4	416.2	423.2	429.0	430.3

Name: *cis*–Octadecafluorodecahydronaphthalene
Formula: $C_{10}F_{18}$

CAS–RN: 60433–11–6
Group No.: 21–031
Molar Mass: 462.08

TABLE 21.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81ZHO/KOS1	269.5–300.6	6	nosp	99.57	melpt	C_{sat}	BSAO	79ZHO/KOS

TABLE 21.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	6	6	0.157	4.17–2	0.08	4.83–5	1
Temp. range K		A_1	A_2				Level of uncertainty
269.5–300.6		2.82565+1	8.65756				IV

TABLE 21.31.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	0.929	0.934	0.945	0.960	0.973	0.976
C_{sat} (J K^{-1}mol^{-1})	429.3	431.6	436.5	443.7	449.6	450.9

Name: *trans*–Octadecafluorodecahydronaphthalene
Formula: $C_{10}F_{18}$

CAS–RN: 60433–12–7
Group No.: 21–032
Molar Mass: 462.08

TABLE 21.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81ZHO/KOS1	296.6–306.1	5	nosp	99.46	melpt	C_{sat}	BSAO	79ZHO/KOS

TABLE 21.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	5	0.241	6.55–2	0.12	9.61–5	1
Temp. range K		A_1	A_2				Level of uncertainty
296.6–306.1		2.06769+1	1.10978+1				IV

TABLE 21.32.4. Recommended values of heat capacities

Temp. (K)	295	298.15	300	305
c_{sat} (J K^{-1}g^{-1})	0.961	0.967	0.971	0.981
C_{sat} (J K^{-1}mol^{-1})	444.1	447.0	448.7	453.3

Name: 2,2',3,3',4,4',5,5',6,6'–Decafluoro–1,1'–biphenyl
Formula: $C_{12}F_{10}$

CAS–RN: 434–90–2
Group No.: 21–033
Molar Mass: 334.12

TABLE 21.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71PAU/RAK	347.5–349.8	3	nosp	99.93	melpt	C_p	BSAO	69PAU/LAV2

TABLE 21.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.001	4.36–4	0.00	2.54–6	0
Temp. range K		A_1	A_2				Level of uncertainty
347.5–349.8		4.15903+1	2.14082				IV

TABLE 21.33.4. Recommended values of heat capacities

Temp. (K)	348	350
c_p (J K^{-1}g^{-1})	1.220	1.221
C_p (J K^{-1}mol^{-1})	407.7	408.1

22. Chlorine Derivatives

The chlorine family contains 49 compounds, 8 of which have data at only one temperature.

No single laboratory specifically focused its attention on the heat capacities of chlorinated compounds. The largest number of chlorinated organic compounds for which heat capacity data were reported (15 substances) were those of Kurbatov (48KUR) from PTIL, however, these data appear to be of low reliability due to the limits of the calorimeter used and due to the uncertain quality of samples studied. Therefore, the data of Kurbatov have been included only in those cases when no other more reliable data were available or when it allowed extension of the temperature interval of the recommended data. The same applied to the data of the German laboratories (*81VON, *87SCH) measured in the late 1800's.

Three sets of data from UCB (40PIT, 48GOR/GIA, 56LI/PIT) and three sets from CIUG (67LEB/RAB2, 78MOS/RAB, 86NOV/RAB) were considered to be high quality data. In the range of higher temperatures, up to about 350 K, the values used were reported from GPI (67RAS/GAN) to have an error of 0.7 %. For two compounds, the data from UCE (57HAR/MOE) with a reported error of 0.5 % have been selected. Also, three compounds measured at ICLO (55STA/TUP) having an uncertainty of 1.0 % were included in the final selection.

Various low molar mass chlorinated hydrocarbons are used as common solvents. It is surprising that despite a large number of measurements, it is difficult to find reliable and consistent data. As an example, for tetrachloromethane, where data from 34 different sources were collected, it is difficult to deduce what is the real dependence of $C_p = f(T)$. Several authors (36LOR/BLA, 44HIC/HOO, 55STA/TUP, 89PET/PES) have found a minimum in the C_p versus temperature curve but each of them reported a different temperature (in the range between 254 to 304 K). There is a real possibility for the existence of a minimum as a similar variation of C_p with temperature was observed for other chlorinated methanes and tetrafluoromethane. A detailed discussion regarding minima on heat capacity curves can be found in the reference (93ZAB/BUR). In the hope of obtaining meaningful recommended values from inconsistent measurements for tetrachloromethane, the data from five sources (and several additional one point measurements) have been simultaneously correlated. The situation was not much better for trichloromethane where the data from the references (55STA/TUP, 57HAR/MOE, 67RAS/GAN) are consistent only to about 1.5 % and the minimum on the C_p curve near 278 K was reported only in the reference (86ALP/PES) from work at IKNR.

For dichloromethane, two data sets were obtained from work at KITH (37PER, 40RIE) both with an error estimated by us to be 1.5 %. They have been, however, discarded and the preference has been given to more recent measurements from CIUG (78MOS/RAB) with a reported error 0.3 %.

No heat capacity data for chloromethane were published after 1940. Both accurate data from PSC (40MES/AST),less reliable data from the Engineering Committee of the Board, London (24SHO), and data from NPLT (40AWB/GRI) have been combined and included to give recommended values over the largest temperature interval possible.

An error of 0.3 % was claimed for the data on tetrachloroethene and reported by CIUG (86NOV/RAB) over the interval from 253 to 300 K; however, at 298 K the C_p data obtained from excess heat capacity measurements (82GRO/ING, 89WIL/LAI) differ by more than 7 %. The data for 1,1-dichloroethene from DCM (59HIL/MCD) are considered to be highly reliable as well as the data for 1,1,1-trichloroethane from NPLT (73AND/CON). The data obtained from the simultaneous measurements of C_p and dielectric constant at PUP (50CRO/SMI) were omitted because of their uncertain reliability for 1,1,1-trichloroethane, but had to be considered for 1,1,2-trichloroethane because it was the only available data source. We expect the error to be between 1 and 2 %.

1,2-Dichloroethane is a frequently measured compound where the data from three sources (40PIT1, 55STA/TUP, 67RAS/GAN) have been supplemented by data for pure components obtained as part of excess heat capacity measurements at the Technological University, Delft, Netherlands (55RUI2) and at UWA (69WIL/SCH).

Most heat capacity measurements for chlorinated benzenes come from the old literature with the exception of the source (74PET/TER) which reports data for 1,2,4-trichlorobenzene; however, the reliability and accuracy appear to be low. Several data sources are available for chlorobenzene at 298 K from measurements on pure components as part of excess heat capacity studies. The temperature dependence for chlorobenzene was reported in the references (37STU) from JHUB and (90RAO/RUJ) from IISB. The latter source has not been considered in the final selection of recommended values because the real uncertainty of the data seems to be much higher than the claimed error 4 %.

Name: Tetrachloromethane
Formula: CCl_4

CAS–RN: 56–23–5
Group No.: 22–001
Molar Mass: 153.82

TABLE 22.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
12SCH2		293.1–323.1	3	nosp	not specified	C_p	BSIO	12SCH1
22LAT		253.8–290.0	3	2.00	not specified	C_p	BSIO	20GIB/LAT
24WIL/DAN		303.0–331.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
25WIL/DAN		293.1–333.1	5S	nosp	not specified	C_p	BSAO	24WIL/DAN
33KOL/UDO	N	288.3	1	nosp	not specified	C_p	BSIT	34KOL/UDO2
36LOR/BLA		260.0–330.0	8S	1.50	not specified	C_p	DSIO	26AND/LYN
37STU		260.0–320.0	7S	nosp	not specified	C_p	BDHO	37STU
37VOL		298.1	1	nosp	not specified	C_p	BSIO	37VOL
39PHI		301.1	1	nosp	not specified	C_p	BSIO	49WEI
41ZHD		278.6–319.2	3	nosp	not specified	C_p	BSIT	34KOL/UDO2
44HIC/HOO		253.8–298.5	13	nosp	99.98 melpt	C_p	BSIO	38HIC
48KUR		299.1	1	nosp	not specified	C_{avg}	DSIO	47KUR
49TSC/RIC3		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
55STA/TUP		295.9–338.8	7	1.00	not specified	C_p	BSAO	55STA/TUP
57HAR/MOE		254.4–303.3	6	0.50	not specified	C_p	BSIO	57HAR/MOE
67GRA		308.1–338.1	7	1.00	not specified	C_p	BSIO	67GRA
67RAS/GAN		293.1–333.1	3S	0.50	not specified	C_p	BSAO	67RAS/GAN
71DES/BHA		298.1–318.1	3S	nosp	not specified	C_p	BSIO	56MUR/VAN
71VAN		255.0–300.0	10S	nosp	99.97 chrom	C_{sat}	BSAO	72VAN
72ARE/VAN		252.6–256.1	3	nosp	99.97 melpt	C_p	BSAO	72VAN
72REC/SAD		298.1–298.1	2	0.30	not specified	C_p	BSIO	70REC
73SUB/RAJ		298.1–323.1	3	0.30	not specified	C_p	BSIO	64MOE/THO
74WIL/ZET		273.1–323.1	6	nosp	not specified	C_p	BSAO	64ARN1
75GRO/BEN		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
76FOR/BEN1		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
78GRO/WIL		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
79GRO/HAM		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
79WIL/FAR		298.1	1	0.30	99.5 chrom	C_p	FSIT	71PIC/LED
81ATA/ELS		293.1	1	2.50	not specified	C_p	BDHO	81ATA/ELS
82TAN		293.1–303.1	3	nosp	99.99 chrom	C_p	FSIT	71PIC/LED
85NKI/CHA		298.0	1	0.30	not specified	C_p	FSIT	71PIC/LED
89LAI/ROD		298.1	1	nosp	99.5 anal	C_p	FSIT	71PIC/LED
89PET/PES		258.1–318.1	4	nosp	not specified	C_p	BSAO	83KUK/KOR

33KOL/UDO same datum in 34KOL/UDO2

TABLE 22.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
+/–								
				Selected data				
44HIC/HOO	253.8–298.5	13	0.50#	0.919	7.24–2	0.46	5.49–3	1
55STA/TUP	295.9–338.8	7	1.00	0.790	1.27–1	0.79	1.22–1	7
67RAS/GAN	293.1–333.1	3	0.50	0.833	6.68–2	0.42	5.93–2	3
73SUB/RAJ	298.1–323.1	3	0.30	1.494	7.07–2	0.45	–6.89–2	–3
74WIL/ZET	273.1–323.1	6	0.30#	0.607	2.88–2	0.18	2.50–2	5
75GRO/BEN	298.1	1	0.30	0.863	4.11–2	0.26	4.11–2	1
76FOR/BEN1	298.1	1	0.30	0.428	2.03–2	0.13	–2.03–2	–1
76FOR/BEN2	298.1	1	0.30	0.504	2.39–2	0.15	–2.39–2	–1
78GRO/WIL	298.1	1	0.30	0.029	1.38–3	0.01	1.38–3	0
79GRO/HAM	298.1	1	0.30	0.029	1.38–3	0.01	1.38–3	0
79WIL/FAR	298.1	1	0.30	0.504	2.39–2	0.15	–2.39–2	–1
82TAN	293.1–303.1	3	0.30#	0.546	2.59–2	0.16	–2.58–2	–3
				Rejected data				
12SCH2	(1.00, 6.07, 2.94–1, 1)			22LAT	(1.60–1, 1.01, 1.60–1, 2)			
24WIL/DAN	(3.57–1, 2.23, 2.86–2, 1)			25WIL/DAN	(2.77–1, 1.74, –4.64–2, –3)			
33KOL/UDO	(5.78–1, 3.80, –5.78–1, –1)			36LOR/BLA	(2.78–1, 1.74, 4.65–2, 2)			
37STU	(1.12–1, 0.71, 4.45–2, 3)			37VOL	(1.69–1, 1.06, 1.69–1, 1)			
39PHI	(1.86–1, 1.16, 1.86–1, 1)			41ZHD	(1.95–1, 1.22, 6.62–2, 1)			
48KUR	(3.28–1, 2.12, –3.28–1, –1)			49TSC/RIC3	(3.55–1, 2.19, 3.55–1, 1)			
57HAR/MOE	(1.00–1, 0.64, –9.39–2, –6)			67GRA	(1.91–1, 1.18, 1.88–1, 7)			
71DES/BHA	(1.22–1, 0.76, 6.39–2, 1)			71VAN	(5.53–1, 3.64, –5.52–1, –10)			
72ARE/VAN	(2.12–1, 1.34, 2.11–1, 2)			72REC/SAD	(3.13–1, 2.03, –2.98–1, –2)			
81ATA/ELS	(1.86–1, 1.19, –1.86–1, –1)			85NKI/CHA	(1.62–1, 1.01, 1.62–1, 1)			
89LAI/ROD	(2.15–1, 1.34, 2.15–1, 1)			89PET/PES	(4.54–1, 2.78, 4.11–1, 4)			

TABLE 22.1.3. Parameters of regression polynomial

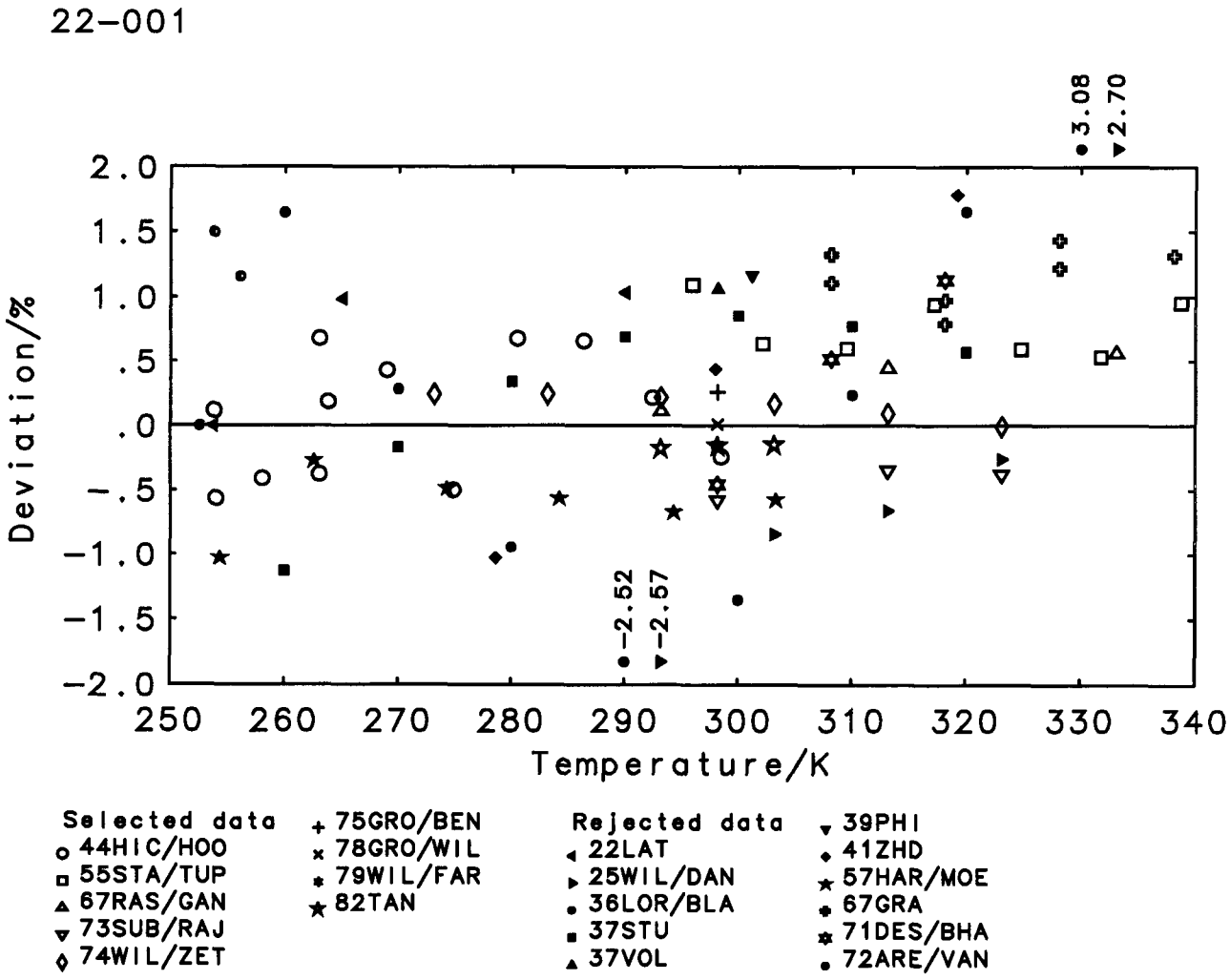
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	116	41	0.869	7.60–2	0.48	2.31–2	8
Temp. range K		A_1	A_2	A_3			Level of uncertainty
253.8–338.8		1.62691+1	–7.50981–1	2.01666–1			IV

TABLE 22.1.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	0.848	0.849	0.850	0.851	0.853	0.855	0.856
C_p (J K^{-1}mol^{-1})	130.4	130.6	130.7	130.9	131.3	131.6	131.6
Temp. (K)	310	320	330	340			
c_p (J K^{-1}g^{-1})	0.858	0.861	0.864	0.867			
C_p (J K^{-1}mol^{-1})	132.0	132.5	132.9	133.4			

TABLE 22.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	116	41	0.951	6.74–2	0.43	4.91–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
253.8–338.8	556.40	7.24295	3.12242	1.24136+1	4.20029		IV



Name: Trichloromethane
Formula: $CHCl_3$

CAS–RN: 67–66–3
Group No.: 22–002
Molar Mass: 119.38

TABLE 22.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
12SCH1		223.1–328.1	9	nosp	not specified		C_p	BSIO	12SCH1
21TRE		295.5–321.8	7	nosp	not specified		C_p	BSIO	49WEI
24WIL/DAN		295.0–318.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
25WIL/DAN		293.1–323.1	4S	nosp	not specified		C_p	BSAO	24WIL/DAN
39PHI		303.5	1	nosp	not specified		C_p	BSIO	49WEI
47SKU		293.1	1	0.30	not specified		C_p	BSAO	47SKU
48KUR		252.9–305.8	4	nosp	not specified		C_{avg}	DSIO	47KUR
49TSC/RIC3		293.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
55STA/TUP		284.0–329.0	11	1.00	not specified		C_p	BSAO	55STA/TUP
57HAR/MOE		245.9–303.2	8	0.50	not specified		C_p	BSIO	57HAR/MOE
67RAS/GAN		293.1–333.1	3S	0.50	not specified		C_p	BSAO	67RAS/GAN
85HEP/KOO		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
86ALP/PES	N	258.1–318.1	4	0.20	not specified		C_p	BSAO	83KUK/KOR
89BAR/KOO1		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
89BAR/KOO2		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
89ING		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
90YAM/OGA		298.1	1	nosp	99.97	chrom	C_p	FSIO	85OGA
91GRO/ROU		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

86ALP/PES same data in 89PET/PES and 90ALP/PES

TABLE 22.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
55STA/TUP	284.0–329.0	11	1.00	0.930	1.29–1	0.93	–8.90–2	–5
57HAR/MOE	245.9–303.2	8	0.50	0.973	6.60–2	0.49	–3.27–2	–4
67RAS/GAN	293.1–333.1	3	0.50	3.201	2.25–1	1.60	2.05–1	3
89BAR/KOO1	298.1	1	0.50#	0.163	1.12–2	0.08	1.12–2	1
89BAR/KOO2	298.1	1	0.50#	0.143	9.81–3	0.07	9.81–3	1
89ING	298.1	1	0.50#	0.025	1.70–3	0.01	1.70–3	1
90YAM/OGA	298.1	1	0.50#	0.713	4.88–2	0.36	–4.88–2	–1
91GRO/ROU	298.1	1	0.50#	0.713	4.88–2	0.36	–4.88–2	–1
				Rejected data				
12SCH1	(4.10–1, 2.94, 3.65–1, 6)			21TRE	(1.27–1, 0.91, 5.58–2, 3)			
24WIL/DAN	(2.53–1, 1.79, 2.52–1, 3)			25WIL/DAN	(3.28–1, 2.28, 3.16–1, 4)			
39PHI	(3.00, 17.84, 3.00, 1)			47SKU	(3.85–1, 2.74, 3.85–1, 1)			
48KUR	(3.72–1, 2.74, 3.95–2, 0)			49TSC/RIC3	(5.65–1, 3.97, 5.65–1, 1)			
85HEP/KOO	(6.20–2, 0.45, –6.20–2, –1)			86ALP/PES	(3.91–1, 2.80, 3.02–1, 4)			

TABLE 22.2.3. Parameters of regression polynomial

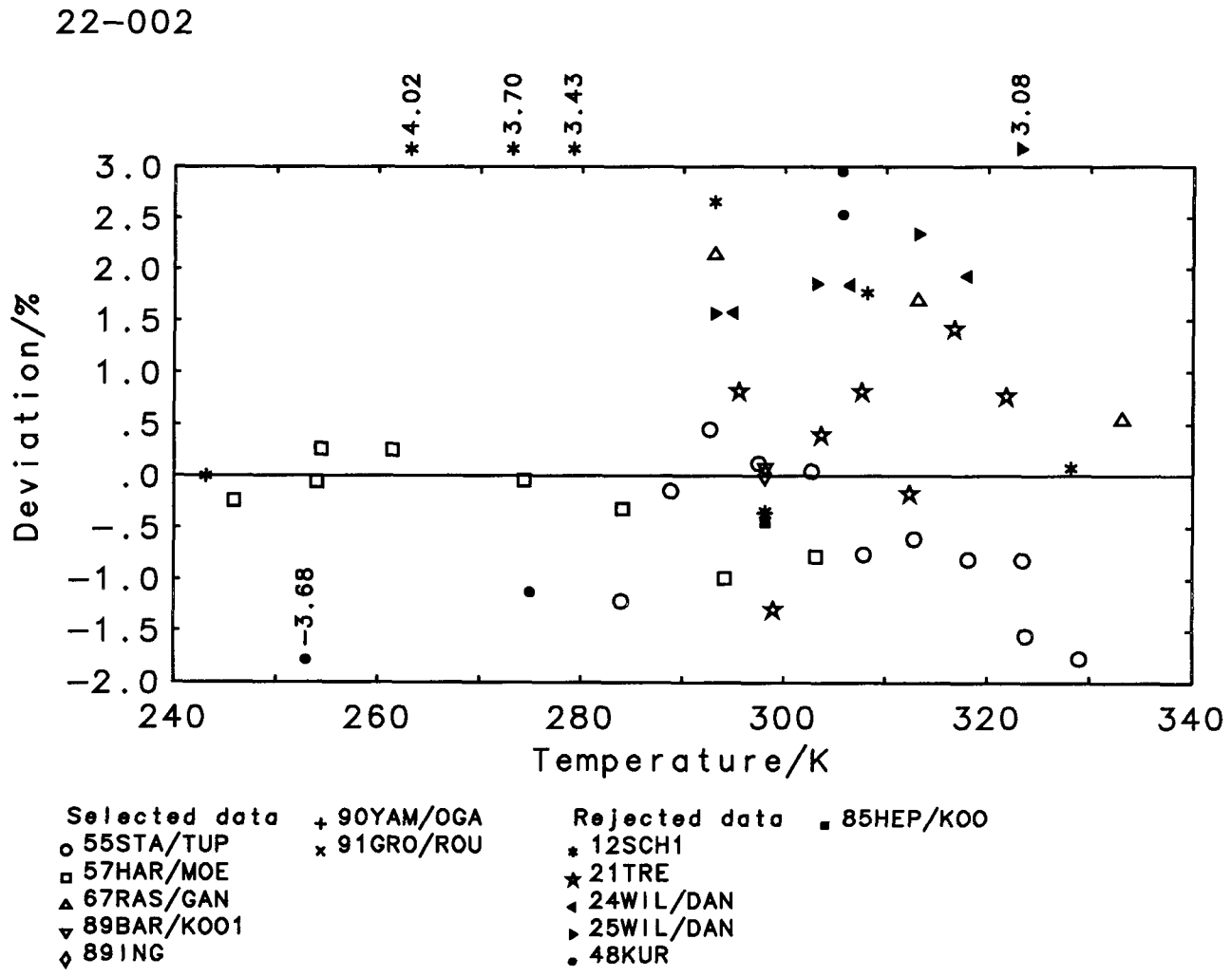
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	27	1.427	1.25–1	0.90	–2.59–2	–5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
245.9–333.1		1.78697+1	–4.18738	9.39942–1			V

TABLE 22.2.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	0.92	0.92	0.93	0.93	0.94	0.94	0.95
C_p ($J K^{-1} mol^{-1}$)	110	110	111	112	112	112	113
Temp. (K)	**298.15**	**300**	**310**	**320**	**330**		
c_p ($J K^{-1} g^{-1}$)	0.96	0.96	0.97	0.98	1.00		
C_p ($J K^{-1} mol^{-1}$)	114	114	116	117	119		

TABLE 22.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	27	1.499	1.17–1	0.84	4.41–4	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
245.9–333.1	536.40	2.94568	2.39978	1.02086+1	9.03939–1		V



Name: Dichloromethane
Formula: CH_2Cl_2

CAS–RN: 75–09–2
Group No.: 22–003
Molar Mass: 84.93

TABLE 22.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
37PER1	N	215.1–292.4	15	0.40	not specified		C_p	BSIO	37PER1
40RIE	N	226.3–313.9	12	nosp	not specified		C_{sat}	BSIO	39RIE3
48KUR		241.0–299.9	4	nosp	not specified		C_{avg}	DSIO	47KUR
78MOS/RAB		182.6–301.0	30	0.30	99.97	melpt	C_p	BSAO	76LEB/LIT

37PER1 same data in 37PER2
40RIE same data in 41RIE1

TABLE 22 3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
78MOS/RAB	182.6–301.0	29	0.30	0.580	2.02–2	0.17	7.08–5	2
				Rejected data				
37PER1	(1.94–1, 1.64, 1.64–1, 13)			40RIE	(2.11–1, 1.78, 1.06–1, 5)			
48KUR	(2.45, 17.00, 2.41, 4)							

TABLE 22.3.3. Parameters of regression polynomial

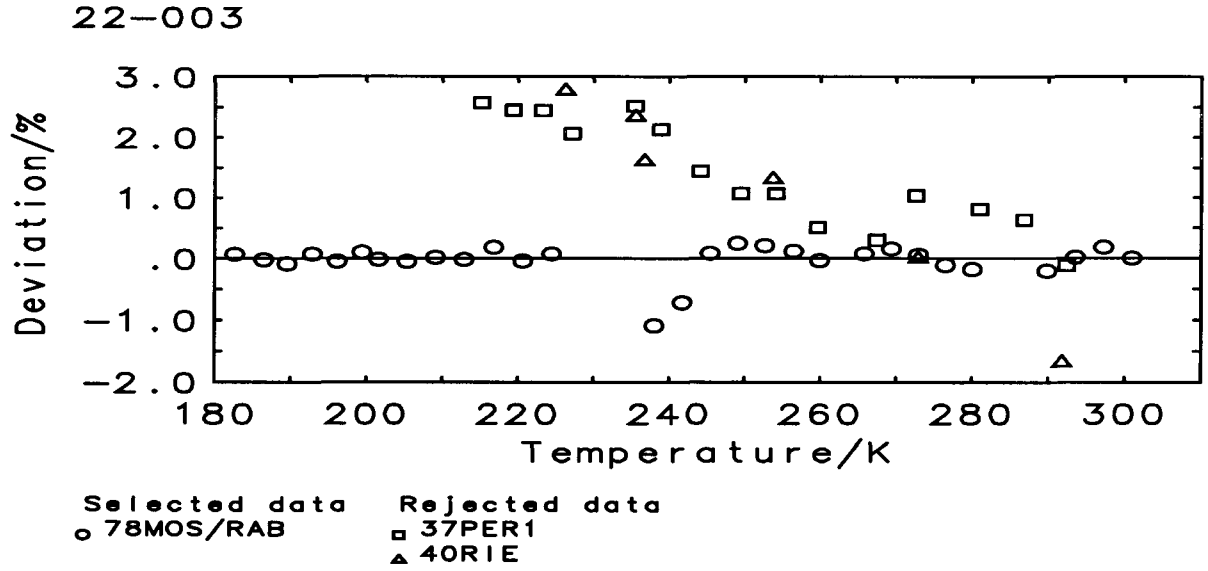
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	61	29	0.625	2.17–2	0.19	7.08–5	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
182.6–301.0		8.44513	6.28476	–3.75910	6.98459–1		III

TABLE 22.3.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.141	1.136	1.132	1.129	1.127	1.127	1.129
C_p (J K^{-1}mol^{-1})	96.88	96.50	96.16	95.90	95.74	95.72	95.88
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.133	1.140	1.151	1.155	1.165	1.184	1.202
C_p (J K^{-1}mol^{-1})	96.25	96.86	97.76	98.11	98.97	100.5	102.1
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.207						
C_p (J K^{-1}mol^{-1})	102.5						

TABLE 22.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	61	17	0.821	2.84–2	0.25	1.15–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
220.6–301.0	510.00	6.64132+1	2.09089+1	−1.05361+1	5.27374+1		III



Name: Chloromethane
Formula: CH_3Cl

CAS–RN: 74–87–3
Group No.: 22–004
Molar Mass: 50.49

TABLE 22.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
24SHO	243.1–313.1	8	nosp	not specified	C_{sat}	BDHO	24SHO
28EUC/HAU	190.0–240.0	6S	nosp	not specified	C_{sat}	BSIO	28EUC/HAU
40AWB/GRI	243.1–303.1	7S	1.00	99.9998 anal	C_{sat}	BSAO	40AWB/GRI
40MES/AST	182.2–249.7	10	0.50	not specified	C_p	BSIO	36AST/MES

TABLE 22.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
24SHO	243.1–313.1	8	1.00#	0.789	7.53–2	0.79	3.66–2	4
40AWB/GRI	243.1–303.1	7	1.00	0.395	3.73–2	0.40	1.67–2	3
40MES/AST	182.2–249.7	10	0.50	0.521	2.35–2	0.26	–9.84–3	0
				Rejected data				
28EUC/HAU	(9.36–2, 1.05, 1.03–2, 2)							

TABLE 22.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	25	0.632	5.25–2	0.55	1.25–2	7
C_{sat}	31	25	0.662	5.54–2	0.59	1.32–2	7

Temp. range K	A_1	A_2	A_3	Level of uncertainty
182.2–313.1	1.30804+1	–4.10065	1.01114	IV
182.2–313.1	1.26596+1	–3.69710	9.14966–1	IV

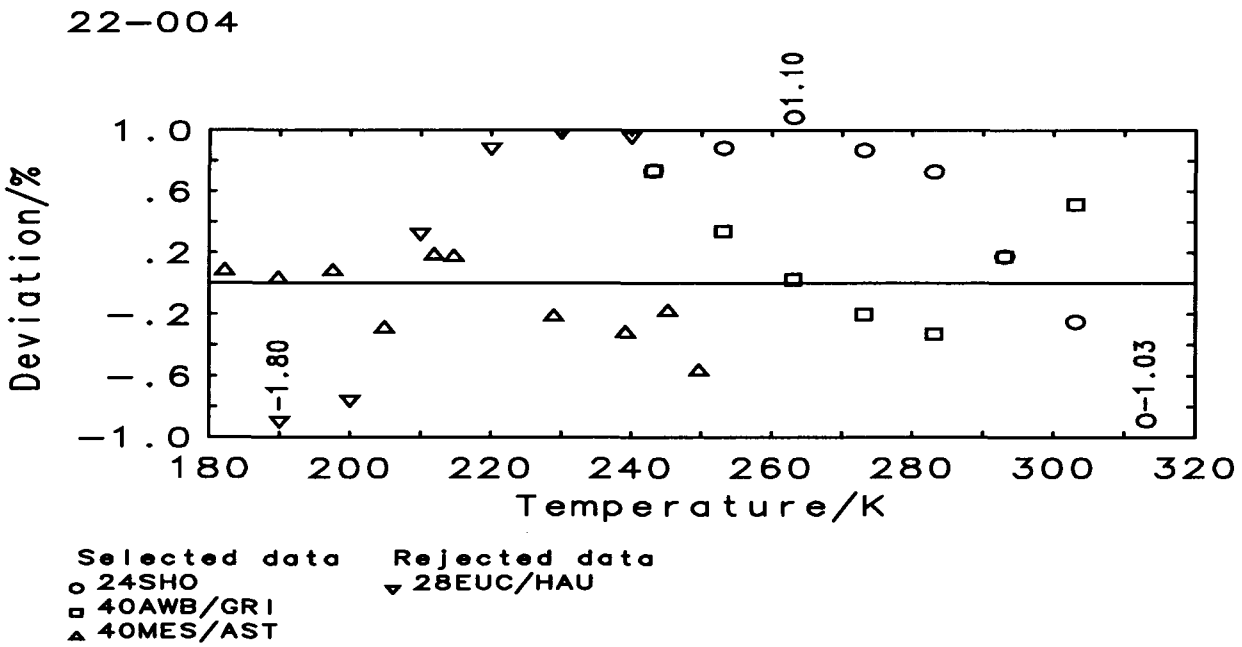
TABLE 22.4.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1} g^{-1}$)	1.478	1.472	1.470	1.470	1.474	1.482	1.493
C_p ($J K^{-1} mol^{-1}$)	74.63	74.33	74.20	74.23	74.44	74.81	75.35
c_{sat} ($J K^{-1} g^{-1}$)	1.477	1.472	1.470	1.471	1.475	1.482	1.492
C_{sat} ($J K^{-1} mol^{-1}$)	74.58	74.32	74.21	74.25	74.45	74.80	75.30
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	1.507	1.524	1.545	1.552	1.569	1.596	1.621
C_p ($J K^{-1} mol^{-1}$)	76.06	76.94	77.99	78.35	79.20	80.59	81.84
c_{sat} ($J K^{-1} g^{-1}$)	1.504	1.520	1.539	1.546	1.561	1.586	1.609
C_{sat} ($J K^{-1} mol^{-1}$)	75.96	76.76	77.72	78.05	78.83	80.09	81.23
Temp. (K)	300	310					
c_p ($J K^{-1} g^{-1}$)	1.627	1.661					
C_p ($J K^{-1} mol^{-1}$)	82.14	83.85					
c_{sat} ($J K^{-1} g^{-1}$)	1.614	1.645					
C_{sat} ($J K^{-1} mol^{-1}$)	81.51	83.07					

TABLE 22.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	22	1.043	5.80–2	0.62	–6.15–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
204.9–313.1	416.25	–5.89496–1	3.84573–1	7.56995	2.25904–1	IV



Name: Tetrachloroethene
Formula: C_2Cl_4

CAS–RN: 127–18–4
Group No.: 22–005
Molar Mass: 165.83

TABLE 22.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	317.7–346.1	3S	nosp	not specified		C_{avg}	DSIO	*81VON
13HER/RAT	293.1	1	nosp	not specified		C_p	DSIO	22HER/SCH
48KUR	319.3–340.9	2	nosp	not specified		C_{avg}	DSIO	47KUR
66SAV	293.0–333.0	eqn	1.20	not specified		C_p	BSIO	66SAV
82GRO/ING	298.1	1	0.30	99.	estim	C_p	FSIT	71PIC/LED
86NOV/RAB	253.1–300.0	14	0.30	99.77	melpt	C_p	BSAO	76LEB/LIT
89WIL/LAI	298.1	1	nosp	99.7	anal	C_p	FSIT	71PIC/LED

TABLE 22.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86NOV/RAB	253.1–300.0	14	0.30	0.221	1.20–2	0.07	1.20–5	–1
				Rejected data				
13HER/RAT	(7.17–1, 3.98, –7.17–1, –1)			66SAV	(2.83, 17.81, –2.83, –1)			
82GRO/ING	(1.36, 7.73, –1.36, –1)			89WIL/LAI	(1.28, 7.24, –1.28, –1)			

TABLE 22.5.3. Parameters of regression polynomial

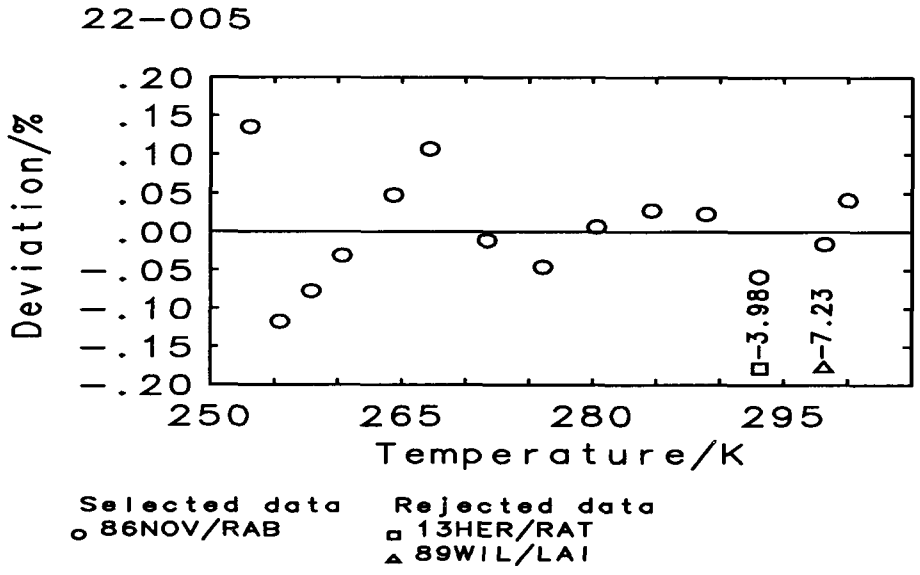
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	14	0.262	1.42–2	0.08	1.20–5	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
253.1–300.0		4.71766+2	–4.72380+2	1.62500+2	–1.84466+1		IV

TABLE 22.5.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	0.895	0.896	0.900	0.911	0.932	0.952	0.956
C_p ($J K^{-1} mol^{-1}$)	148.5	148.7	149.2	151.0	154.6	157.8	158.5

TABLE 22.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	11	0.751	4.10–2	0.23	9.17–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
260.3–300.0	620.20	1.05500+3	3.32726+2	–3.32429+2	8.36292+2		IV



Name: Trichloroethene
Formula: C_2HCl_3

CAS–RN: 79–01–6
Group No.: 22–006
Molar Mass: 131.39

TABLE 22.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
13HER/RAT	293.1	1	nosp	not specified		C_p	DSIO	22HER/SCH
33TRE/WAT	298.1	1	nosp	not specified		C_p	BSIO	49WEI
48KUR	298.9–320.9	3	nosp	not specified		C_{avg}	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1

TABLE 22.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
13HER/RAT	293.1	1	2.00#	0.000	9.54–7	0.00	9.54–7	0
33TRE/WAT	298.1	1	2.00#	0.137	4.12–2	0.27	4.12–2	1
49TSC/RIC3	298.1	1	3.00#	0.204	9.10–2	0.61	–9.10–2	–1

TABLE 22.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	3	0.246	9.99–2	0.67	–1.66–2	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–298.1		1.65317	4.46558				VI

TABLE 22.6.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	0.92	0.95	0.95
C_p ($J K^{-1} mol^{-1}$)	121	124	125

Name: Pentachloroethane
Formula: C_2HCl_5

CAS–RN: 76–01–7
Group No.: 22–007
Molar Mass: 202.29

TABLE 22.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
13HER/RAT	293.1	1	nosp	not specified		C_p	DSIO	22HER/SCH
48KUR	331.2–358.7	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 22.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
13HER/RAT	293.1	1	3.00#	1.127	9.16-1	3.38	9.16-1	1
48KUR	331.2-358.7	3	5.00#	0.692	8.66-1	3.46	-7.30-1	-3

TABLE 22.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	4	0.950	1.01	3.97	-3.19-1	-2
Temp. range K		A_1					Level of uncertainty
293.1-358.7		2.61625+1					VI

TABLE 22.7.4. Recommended values of heat capacities

Temp. (K)	300	320	340	360
c_p ($J K^{-1} g^{-1}$)	1.08	1.08	1.08	1.08
C_p ($J K^{-1} mol^{-1}$)	218	218	218	218

Name: 1,1-Dichloroethene
Formula: $C_2H_2Cl_2$

CAS-RN: 75-35-4
Group No.: 22-008
Molar Mass: 96.94

TABLE 22.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81BER/OGI	N	304.6	1	nosp	not specified		C_{avg}	DSIO	*79BER
59HIL/MCD		157.4-290.9	37	0.25	99.97	melpt	C_p	BSAO	58HIL/KRA

*81BER/OGI average value in temperature range 286-323 K

TABLE 22.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
59HIL/MCD	157.4-290.9	37	0.25	0.918	2.86-2	0.23	1.30-4	-3

TABLE 22.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	37	0.957	2.98–2	0.24	1.30–4	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
157.4–290.9		1.38528+1	–2.12017	6.53036–1			II

TABLE 22.8.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.041	1.041	1.042	1.045	1.048	1.053	1.059
C_p (J K^{-1}mol^{-1})	100.9	100.9	101.0	101.3	101.6	102.1	102.7
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.066	1.074	1.084	1.094	1.105	1.109	1.118
C_p (J K^{-1}mol^{-1})	103.4	104.1	105.0	106.1	107.2	107.5	108.4
Temp. (K)	290	298.15					
c_p (J K^{-1}g^{-1})	1.132	1.144					
C_p (J K^{-1}mol^{-1})	109.7	110.9					

TABLE 22.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	37	1.143	3.53–2	0.29	1.82–4	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
157.4–290.9	491.30	1.04006+1	5.12849	6.88139	5.27314		III

Name: 1,2–Dichloroethene
Formula: $C_2H_2Cl_2$

CAS–RN: 540–59–0
Group No.: 22–009
Molar Mass: 96.94

TABLE 22.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48KUR	N	265.2–306.5	3	nosp	not specified		C_{avg}	DSIO	47KUR

48KUR mixture of stereoisomers (according to n.b.t.)

TABLE 22.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.112	7.50–2	0.56	3.03–4	1
Temp. range K		A_1	A_2				Level of uncertainty
265.2–306.5		5.52070	2.63049				VI

TABLE 22.9.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c ($J K^{-1} g^{-1}$)	1.08	1.09	1.11	1.13	1.15	1.15	1.17
C ($J K^{-1} mol^{-1}$)	105	106	107	109	111	112	114

Name: (*E*)–1,2–Dichloroethene
Formula: $C_2H_2Cl_2$

CAS–RN: 156–60–5
Group No.: 22–010
Molar Mass: 96.94

TABLE 22.10.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34MEH2	N	288.15	1.163	1.50	not specified		C_p	BSIO	49WEI

34MEH2 isomer not specified, n.b.t. given for Z–isomer

Name: (Z)–1,2–Dichloroethene
Formula: $C_2H_2Cl_2$

CAS–RN: 156–59–2
Group No.: 22–011
Molar Mass: 96.94

TABLE 22.11.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34MEH2	N	288.15	1.176	1.50	not specified		C_p	BSIO	49WEI

34MEH2 isomer not specified, n.b.t. given for *E*–isomer

Name: 1,1,1,2–Tetrachloroethane
Formula: $C_2H_2Cl_4$

CAS–RN: 630–20–6
Group No.: 22–012
Molar Mass: 167.85

TABLE 22.12.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78GUN/HEA	N	295.00	1.120	nosp	99.96	chrom	C_p	not specified	

78GUN/HEA the origin of data unclear

Name: 1,1,2,2–Tetrachloroethane
Formula: $C_2H_2Cl_4$

CAS–RN: 79–34–5
Group No.: 22–013
Molar Mass: 167.85

TABLE 22.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
13HER/RAT	293.1	1	nosp	not specified	C_p	DSIO	22HER/SCH
34MEH1	289.1	1	1.50	not specified	C_p	BSIO	49WEI
48KUR	308.6–353.6	6	nosp	not specified	C_{avg}	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
82KOS/KOL	233.6–296.5	12	nosp	99.4 melpt	C_{sat}	BSAO	79ZHO/KOS
89PRA/RAJ	318.1–333.1	4	3.00	not specified	C_p	BDHT	89PRA/RAJ
89WIL/LAI	298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED

TABLE 22.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48KUR	308.6–353.6	6	5.00#	0.635	6.21–1	3.18	5.16–2	2
82KOS/KOL	233.6–296.5	12	0.40#	0.484	3.85–2	0.19	–1.03–2	0
89WIL/LAI	298.1	1	0.50#	1.973	1.99–1	0.99	1.99–1	1
				Rejected data				
13HER/RAT	(2.68, 11.84, 2.68, 1)			34MEH1	(2.55, 11.33, 2.55, 1)			
49TSC/RIC3	(2.29, 10.28, 2.29, 1)			89PRA/RAJ	(3.80, 22.96, –3.80, –4)			

TABLE 22.13.3. Parameters of regression polynomial

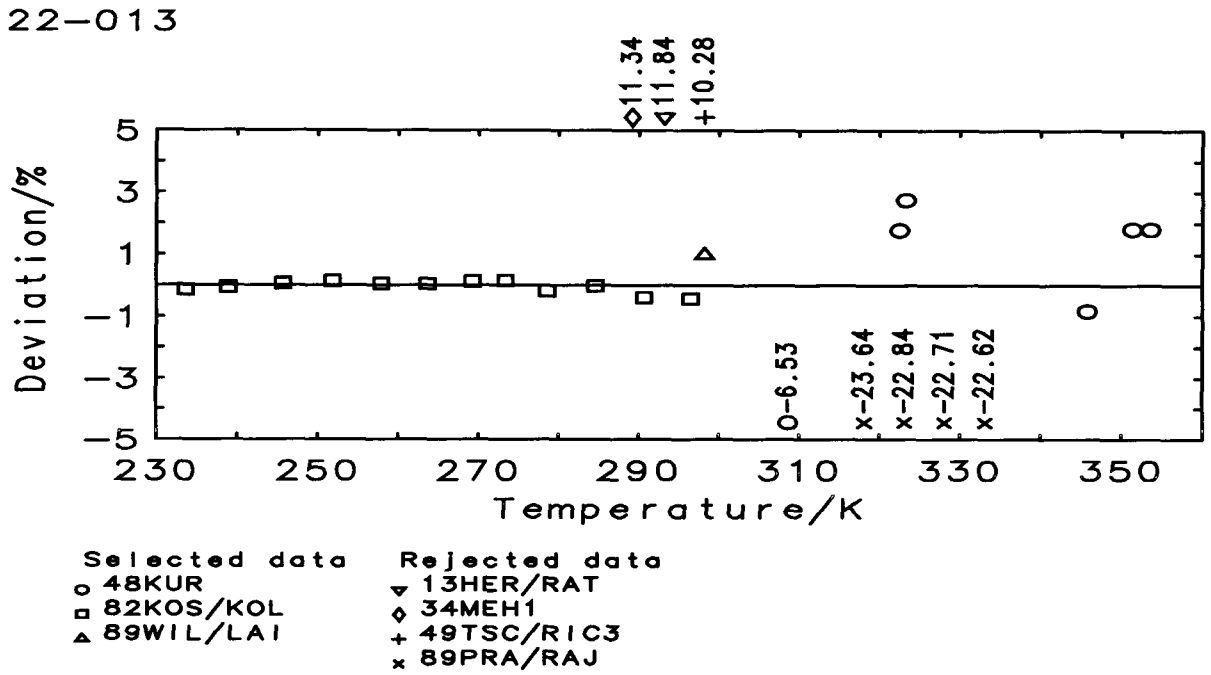
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	26	19	0.755	3.85–1	1.97	2.03–2	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
233.6–353.6		2.66394+1	–5.49537	1.09697			V

TABLE 22.13.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c ($J\,K^{-1}g^{-1}$)	0.98	0.98	0.98	0.98	0.98	0.98	0.99
C ($J\,K^{-1}mol^{-1}$)	164	164	164	165	165	165	166
Temp. (K)	298.15	300	310	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	0.99	0.99	1.00	1.00	1.01	1.02	1.03
C ($J\,K^{-1}mol^{-1}$)	166	167	168	169	170	172	173

TABLE 22.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	26	19	0.841	3.63–1	1.86	9.86–3	11
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
233.6–353.6	626.00	1.67164+2	5.31104+1	–3.59982+1	1.31537+2		V



Name: Chloroethene
Formula: C_2H_3Cl

CAS–RN: 75–01–4
Group No.: 22–014
Molar Mass: 62.50

TABLE 22.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67LEB/RAB2	119.2–300.0	10S	0.50	99.7	melpt	C_{sat}	BSAO	56POP/KOL

TABLE 22.14.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.147	7.58–3	0.07	5.63–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
119.2–240.0		9.72177	8.87961–1	–5.12663–1	9.77939–2		IV
240.0–300.0		–1.53611+1	3.22416+1	–1.35767+1	1.91224		IV

TABLE 22.14.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_{sat} (J K^{-1}g^{-1})	1.359	1.360	1.361	1.361	1.361	1.361	1.361
C_{sat} (J K^{-1}mol^{-1})	84.96	85.01	85.04	85.06	85.06	85.06	85.05
Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.361	1.361	1.361	1.362	1.363	1.364	1.366
C_{sat} (J K^{-1}mol^{-1})	85.05	85.05	85.07	85.10	85.16	85.24	85.37
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.370	1.378	1.381	1.390	1.410	1.432	1.437
C_{sat} (J K^{-1}mol^{-1})	85.62	86.10	86.32	86.90	88.11	89.47	89.83

TABLE 22.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.421	2.17–2	0.21	–2.61–3	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
119.2–300.0	429.70	1.37504+1	3.86185	5.92523	1.22398+1		IV

Name: 1,1,1–Trichloroethane
Formula: $C_2H_3Cl_3$

CAS–RN: 71–55–6
Group No.: 22–015
Molar Mass: 133.40

TABLE 22.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
44RUB/LEV	245.4–299.6	10	2.00	99.7 melpt	C_p	BSAO	41YOS/GAR
50CRO/SMY2	243.1–257.1	6	0.50	not specified	C_p	BDHO	50KUS/CRO
73AND/COU	243.1–310.0	10S	nosp	99.99 melpt	C_p	BSAO	63AND/COU1
88ING	298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
89PRA/RAJ	318.1–333.1	4	3.00	not specified	C_p	BDHT	89PRA/RAJ

TABLE 22.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73AND/COU	243.1–310.0	10	0.20#	0.348	1.19–2	0.07	1.47–5	1
				Rejected data				
44RUB/LEV	(5.69–2, 0.34, –4.37–2, –10)			50CRO/SMY2	(2.10–1, 1.26, –2.08–1, –6)			
88ING	(1.48–1, 0.84, 1.48–1, 1)							

TABLE 22.15.3. Parameters of regression polynomial

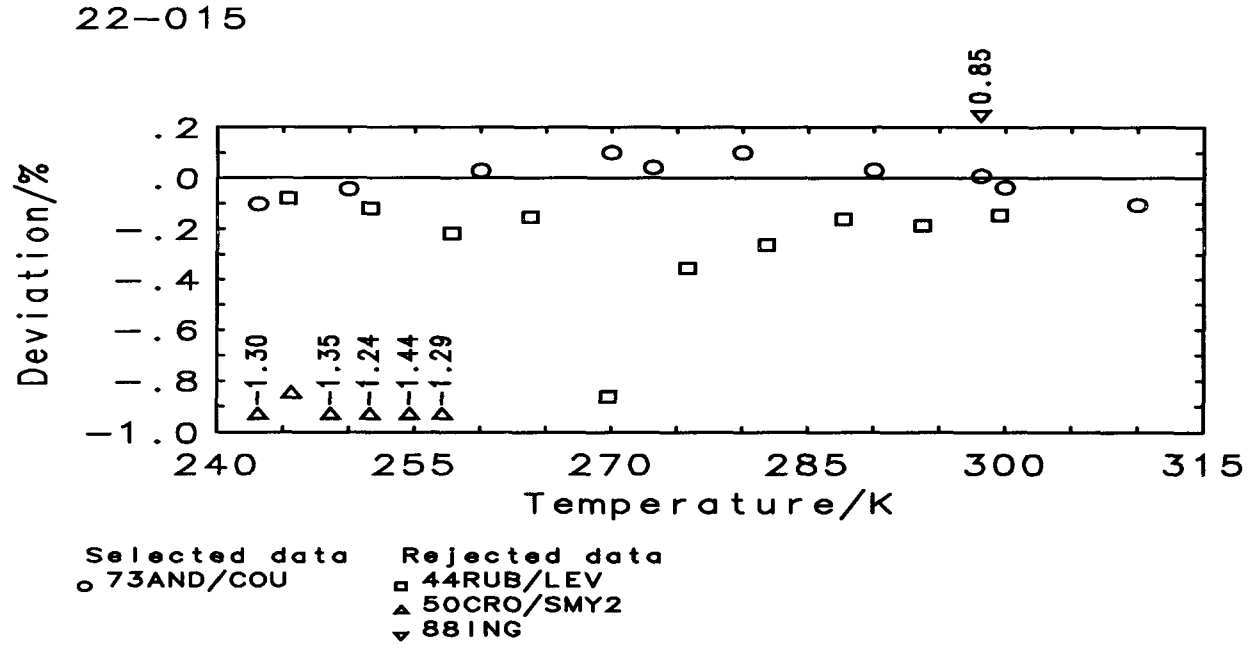
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	10	0.389	1.33–2	0.08	1.47–5	1
Temp. range K		A_1	A_2				Level of uncertainty
243.1–310.0		1.41433+1	1.08096				II

TABLE 22.15.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.050	1.057	1.063	1.066	1.070	1.077	1.082
C_p (J K^{-1}mol^{-1})	140.1	141.0	141.9	142.1	142.8	143.7	144.4
Temp. (K)	300	310					
c_p (J K^{-1}g^{-1})	1.084	1.090					
C_p (J K^{-1}mol^{-1})	144.6	145.5					

TABLE 22.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	10	0.114	3.91–3	0.02	1.72–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
243.1–310.0	545.00	7.01313	7.15455–1	1.19382+1	1.71863+1		II



Name: 1,1,2–Trichloroethane
Formula: $C_2H_3Cl_3$

CAS–RN: 79–00–5
Group No.: 22–016
Molar Mass: 133.40

TABLE 22.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50CRO/SMY2	240.1–251.6	4	1.50	not specified		C_p	BDHO	50KUS/CRO

TABLE 22.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.611	1.57–1	0.92	1.44–3	0

Temp. range K	A_1	A_2	Level of uncertainty
240.1–251.6	1.13833+1	2.35057	V

TABLE 22.16.4. Recommended values of heat capacities

Temp. (K)	240	250
c_p (J K^{-1}g^{-1})	1.06	1.08
C_p (J K^{-1}mol^{-1})	142	144

Name: 1,1–Dichloroethane
Formula: $C_2H_4Cl_2$

CAS–RN: 75–34–3
Group No.: 22–017
Molar Mass: 98.96

TABLE 22.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	297.9–312.3	3S	nosp	not specified		C_{avg}	DSIO	*81VON
48KUR	253.0–309.6	4	nosp	not specified		C_{avg}	DSIO	47KUR
56LI/PIT	177.1–294.3	18	0.20	99.87	melpt	C_p	BSIO	37GIA/EGA

TABLE 22.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56LI/PIT	177.1–294.3	18	0.20	0.595	1.75–2	0.12	4.18–5	–3
				Rejected data				
48KUR	(6.19–1, 4.37, –6.19–1, –1)							

TABLE 22.17.3. Parameters of regression polynomial

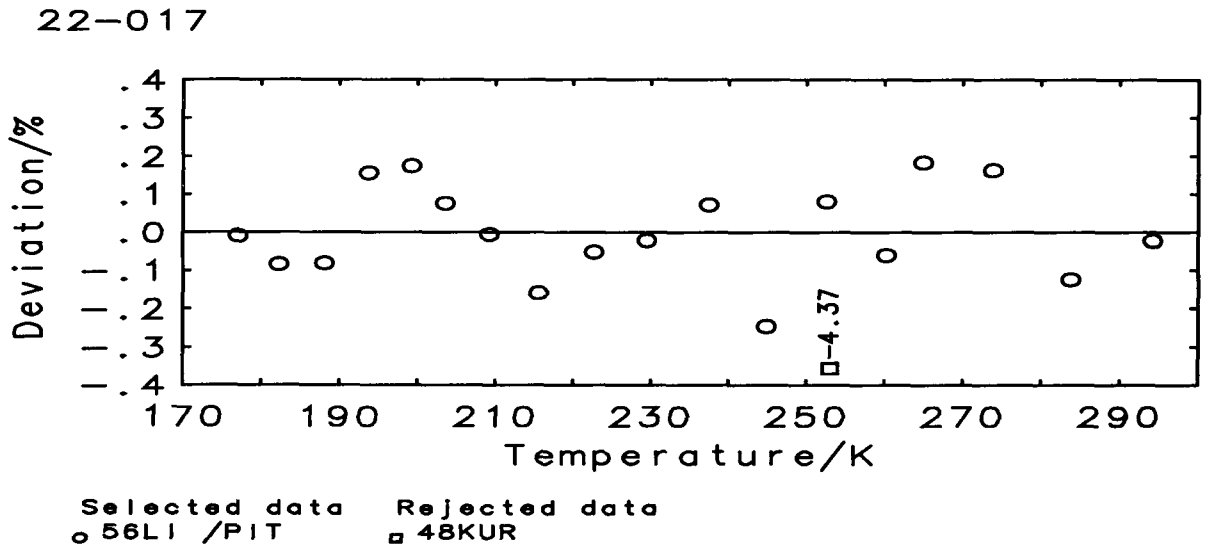
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	18	0.652	1.91–2	0.13	4.18–5	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
177.1–294.3		1.48825+1	–8.54817–1	3.22034–1			II

TABLE 22.17.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.209	1.212	1.215	1.219	1.223	1.228	1.234
C_p (J K^{-1}mol^{-1})	119.6	119.9	120.2	120.6	121.1	121.6	122.1
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.240	1.247	1.254	1.256	1.261	1.270	1.277
C_p (J K^{-1}mol^{-1})	122.7	123.4	124.1	124.3	124.8	125.6	126.4
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.278						
C_p (J K^{-1}mol^{-1})	126.5						

TABLE 22.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	18	0.685	2.02–2	0.14	4.58–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
177.1–294.3	523.00	1.81454	1.86630	1.21488+1	4.41056–1		II



Name: 1,2–Dichloroethane
Formula: $C_2H_4Cl_2$

CAS–RN: 107–06–2
Group No.: 22–018
Molar Mass: 98.96

TABLE 22.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
12SCH1		293.1–323.1	3	nosp	not specified	C_p	BSIO	12SCH1
39RAI	N	240.0–322.0	15	2.00	99.96 melpt	C_p	BDHO	37STU
40PIT1		238.7–307.5	6	0.20	99.942 melpt	C_p	BSIO	28LAT/GRE
48KUR		270.5–322.1	4	nosp	not specified	C_{avg}	DSIO	47KUR
48TSC5		294.1	1	nosp	not specified	C_p	BSIO	48TSC1
48TSC6		294.1	1	nosp	not specified	C_p	BSIO	48TSC1
49TSC/RIC3		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
51SIE/CRU	N	293.1	1	nosp	not specified	C_p	not specified	
55RUI2		280.8–323.7	4	nosp	not specified	C_p	BSIO	55RUI1
55STA/TUP		284.1–348.0	14	1.00	not specified	C_p	BSAO	55STA/TUP
67RAS/GAN		293.1–353.1	4S	0.50	not specified	C_p	BSAO	67RAS/GAN
69WIL/SCH		293.1–313.1	3	0.40	not specified	C_p	BDAO	65FIN/GRU
77WIL/GRO		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
79WIL/FAR		298.1	1	0.30	99.5 melpt	C_p	FSIT	71PIC/LED
79WIL/GRO		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
89PRA/RAJ		318.1–333.1	4	3.00	not specified	C_p	BDHT	89PRA/RAJ
93HAL		298.1	1	0.15	99.9 chrom	C_p	DDCT	74SUU/WAD

39RAI data from a graph only
51SIE/CRU heat of mixing calorimeter used

TABLE 22.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40PIT1	238.7–307.5	6	0.20	1.688	5.12–2	0.34	–7.29–3	–1
55RUI2	280.8–323.7	4	0.50#	0.914	7.18–2	0.46	6.09–2	4
55STA/TUP	284.1–348.0	14	1.00	0.696	1.12–1	0.70	9.21–2	10
67RAS/GAN	293.1–353.1	4	0.50	1.377	1.10–1	0.69	2.84–3	1
69WIL/SCH	293.1–313.1	3	0.40	1.433	8.92–2	0.57	–7.29–2	–3
77WIL/GRO	298.1	1	0.30	0.214	9.96–3	0.06	9.96–3	1
79WIL/FAR	298.1	1	0.30	0.214	9.96–3	0.06	9.96–3	1
79WIL/GRO	298.1	1	0.30	0.111	5.14–3	0.03	5.14–3	1
				Rejected data				
12SCH1	(3.47–1, 2.29, –3.28–1, –3)			39RAI	(3.13–1, 2.08, 3.43–2, 3)			
48KUR	(7.56–1, 5.32, –6.46–1, –4)			48TSC5	(1.70–1, 1.11, –1.70–1, –1)			
48TSC6	(1.45–1, 0.94, –1.45–1, –1)			49TSC/RIC3	(5.31–1, 3.31, 5.31–1, 1)			
51SIE/CRU	(5.11–1, 3.42, –5.11–1, –1)			89PRA/RAJ	(8.90–1, 5.93, –8.89–1, –4)			
93HAL	(5.93–2, 0.38, 5.93–2, 1)							

TABLE 22.18.3. Parameters of regression polynomial

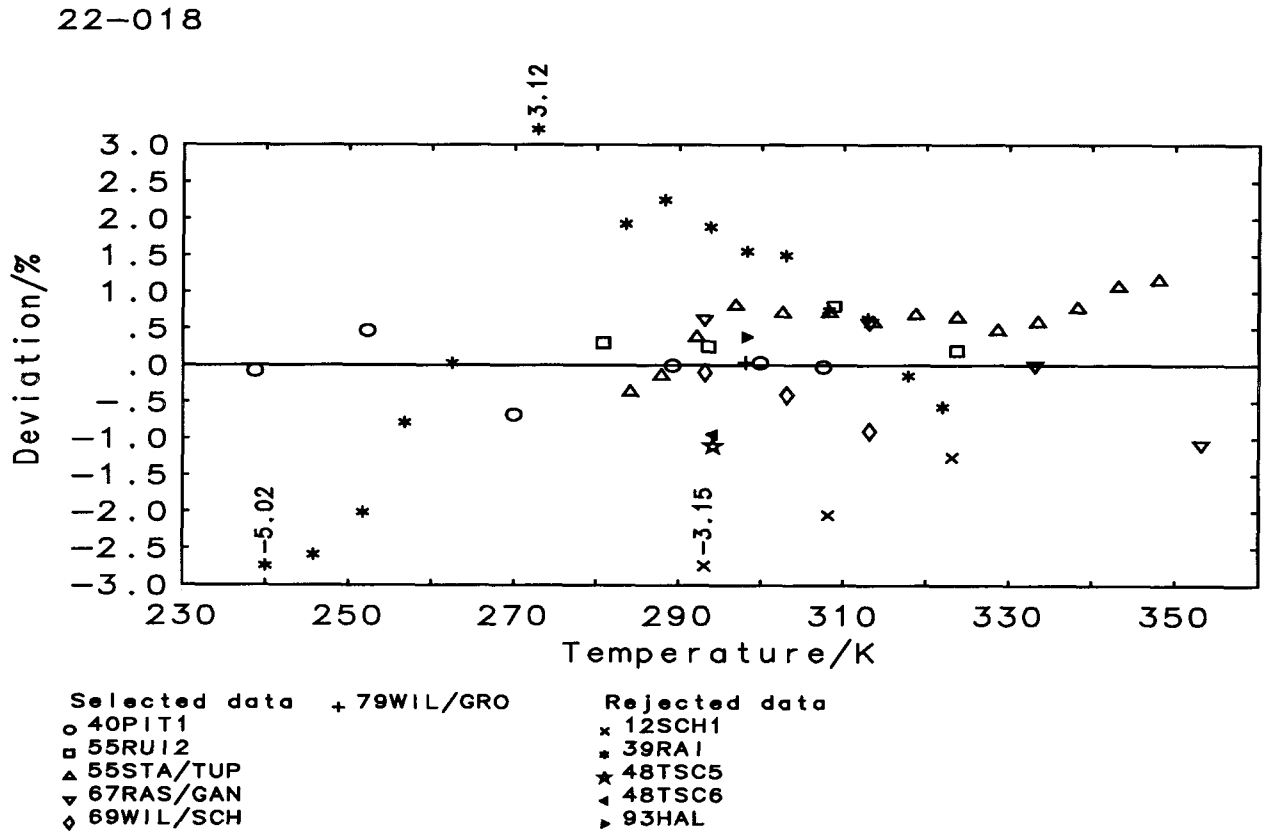
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	34	1.151	9.58–2	0.60	3.84–2	14
Temp. range K		A_1	A_2	A_3			Level of uncertainty
238.7–353.1		1.99782+1	–4.19575	9.03923–1			IV

TABLE 22.18.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	1.270	1.272	1.275	1.280	1.282	1.287	1.295
C_p ($J K^{-1} mol^{-1}$)	125.7	125.9	126.2	126.7	126.9	127.4	128.1
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.303	1.305	1.316	1.328	1.342	1.358	1.375
C_p ($J K^{-1} mol^{-1}$)	128.9	129.1	130.2	131.4	132.8	134.4	136.1

TABLE 22.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	34	1.280	9.27–2	0.58	2.15–2	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
238.7–353.1	561.60	1.34623+1	6.11509	8.73738	7.40930		IV



Name: Chloroethane
Formula: C_2H_5Cl

CAS–RN: 75–00–3
Group No.: 22–019
Molar Mass: 64.51

TABLE 22.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
23JEN/SHO	N	243.1–313.1	14S	nosp	not specified	C_{sat}	FSIO	23JEN/SHO
40RIE	N	224.8–318.1	12	nosp	not specified	C_{sat}	BSIO	39RIE3
48GOR/GIA		139.8–284.5	26	nosp	99.98 melpt	C_p	BSIO	28GIA/WIE1
48KUR		247.1–277.3	3	nosp	not specified	C_{avg}	DSIO	47KUR

23JEN/SHO values calculated from temperature dependence of enthalpy by the authors
40RIE same data in 41RIE1

TABLE 22.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40RIE	224.8–318.1	12	1.50#	1.169	2.22–1	1.75	1.62–1	8
48GOR/GIA	139.8–284.5	26	0.40#	0.466	2.23–2	0.19	–4.99–3	–7
				Rejected data				
23JEN/SHO	(2.28–1, 1.95, –4.36–2, 2)			48KUR		(4.47–1, 3.57, 4.42–1, 3)		

TABLE 22.19.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	55	38	0.817	1.36–1	1.07	4.79–2	1

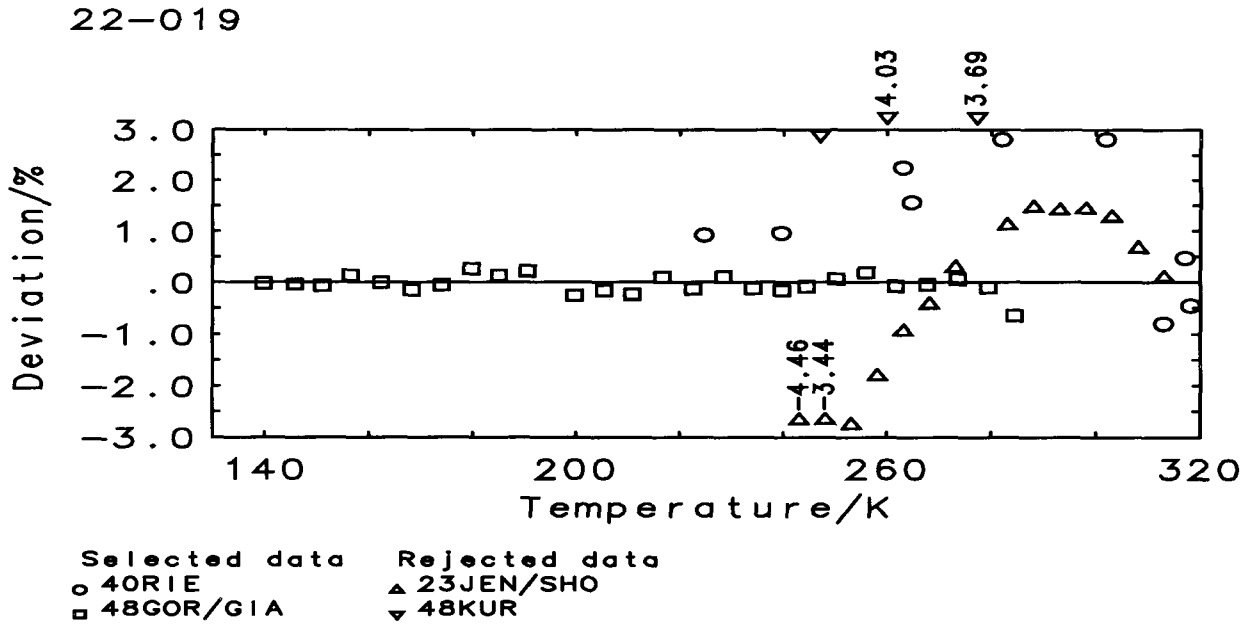
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
139.8–260.0	1.46953+1	–3.66454	1.13262	–4.72340–2	III
260.0–318.1	–5.08597+1	7.19759+1	–2.79598+1	3.68257	V

TABLE 22.19.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p ($J\,K^{-1}g^{-1}$)	1.502	1.493	1.487	1.483	1.481	1.482	1.485
C_p ($J\,K^{-1}mol^{-1}$)	96.91	96.34	95.93	95.67	95.56	95.60	95.77
Temp. (K)	210	220	230	240	250	260	270
c_p ($J\,K^{-1}g^{-1}$)	1.489	1.497	1.506	1.517	1.530	1.546	1.56
C_p ($J\,K^{-1}mol^{-1}$)	96.09	96.55	97.14	97.87	98.73	99.72	101
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	1.57	1.59	1.62	1.65	1.66	1.71	1.78
C_p ($J\,K^{-1}mol^{-1}$)	101	102	104	106	107	110	115

TABLE 22.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	55	32	1.682	1.22–1	0.98	1.53–2	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
174.1–318.1	460.40	8.59220	4.29204	6.93412	4.30017		V



Name: 1,1,1,3–Tetrachloropropane
Formula: $C_3H_4Cl_4$

CAS–RN: 1070–78–6
Group No.: 22–020
Molar Mass: 181.88

TABLE 22.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74KOL/VOR	239.6–288.5	11	nosp	99.82	melpt	C_{sat}	BSAO	62KOL/SER

TABLE 22.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	11	11	0.098	6.83–3	0.03	3.12–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
239.6–288.5		2.59535+1	–3.41993	8.85508–1			III

TABLE 22.20.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.044	1.049	1.054	1.059	1.061	1.066	1.074
C_{sat} (J K^{-1}mol^{-1})	190.0	190.7	191.6	192.7	193.1	193.9	195.2
Temp. (K)	298.15						
c_{sat} (J K^{-1}g^{-1})	1.080						
C_{sat} (J K^{-1}mol^{-1})	196.5						

TABLE 22.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.091	6.34–3	0.03	2.08–6	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
239.6–288.5	571.00	2.00474+1	9.88188	1.24560+1	1.01676+1		III

Name: 3–Chloro–1–propene
Formula: C_3H_5Cl

CAS–RN: 107–05–1
Group No.: 22–021
Molar Mass: 76.53

TABLE 22.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	299.3–312.1	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 22.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.002	9.52–4	0.01	2.38–7	0
Temp. range K		A_1	A_2				Level of uncertainty
299.3–312.1		1.03308+1	1.56868				V

TABLE 22.21.4. Recommended values of heat capacities

Temp. (K)	300	310
c (J K^{-1}g^{-1})	1.63	1.65
C (J K^{-1}mol^{-1})	125	126

Name: 1,2,3–Trichloropropane
Formula: $C_3H_5Cl_3$

CAS–RN: 96–18–4
Group No.: 22–022
Molar Mass: 147.43

TABLE 22.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41NEL/NEW	273.0–333.0	eqn	0.50	not specified		C_p	BSIO	41NEL/NEW
48KUR	320.1–358.9	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 22.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41NEL/NEW	273.0–333.2	8	0.50	0.000	1.51–6	0.00	1.19–6	0
				Rejected data				
48KUR	(7.75–1, 3.58, –7.75–1, –1)							

TABLE 22.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	8	0.000	1.74–6	0.00	1.19–6	0
Temp. range K		A_1	A_2				Level of uncertainty
273.0–333.2		1.72456+1	1.61733				V

TABLE 22.22.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	1.22	1.22	1.23	1.24	1.24	1.25	1.26
C_p ($J K^{-1} mol^{-1}$)	180	180	181	182	183	184	185
Temp. (K)	320	330					
c_p ($J K^{-1} g^{-1}$)	1.26	1.27					
C_p ($J K^{-1} mol^{-1}$)	186	188					

Name: 1,2–Dichloropropane
Formula: $C_3H_6Cl_2$

CAS–RN: 78–87–5
Group No.: 22–023
Molar Mass: 112.99

TABLE 22.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	305.9–359.3	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 22.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	3	3	0.111	1.10–1	0.55	3.03–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
306.0–359.3		5.30569	4.34878				VI

TABLE 22.23.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360
c ($J K^{-1}g^{-1}$)	1.38	1.41	1.45	1.48	1.51	1.54
C ($J K^{-1}mol^{-1}$)	156	160	163	167	171	174

Name: 1,3–Dichloropropane
Formula: $C_3H_6Cl_2$

CAS–RN: 142–28–9
Group No.: 22–024
Molar Mass: 112.99

TABLE 22.24.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
93HAL	298.15	1.390	0.15	99.9	chrom	C_p	DDCT	74SUU/WAD

Name: 2,2–Dichloropropane
Formula: $C_3H_6Cl_2$

CAS–RN: 594–20–7
Group No.: 22–025
Molar Mass: 112.99

TABLE 22.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
72VAN	240.5–266.7	8	0.50	99.72	melpt	C_p	BSAO	72VAN

TABLE 22.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	8	8	0.354	3.20–2	0.18	8.51–5	–2
Temp. range K		A_1	A_2				Level of uncertainty
240.5–266.7		1.54043+1	1.03091				III

TABLE 22.25.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270
c_p ($J K^{-1}g^{-1}$)	1.316	1.323	1.331	1.338
C_p ($J K^{-1}mol^{-1}$)	148.7	149.5	150.4	151.2

Name: 1–Chloropropane
Formula: C_3H_7Cl

CAS–RN: 540–54–5
Group No.: 22–026
Molar Mass: 78.54

TABLE 22.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		299.1–311.6	4S	nosp	not specified		C_{avg}	DSIO	*81VON
48EUC	N	200.0–293.0	4S	nosp	not specified		C_p	not specified	
48KUR		261.9–300.8	2	nosp	not specified		C_{avg}	DSIO	47KUR

48EUC unpublished data measured by A.Landsberg

TABLE 22.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
*81VON	299.1–311.6	4	2.00#	0.484	1.55–1	0.97	–4.90–2	0
48EUC	200.0–293.0	4	1.50#	0.534	1.18–1	0.80	3.09–2	2
			Rejected data					
48KUR	(3.33–1, 2.23, 2.86–1, 2)							

TABLE 22.26.3. Parameters of regression polynomial

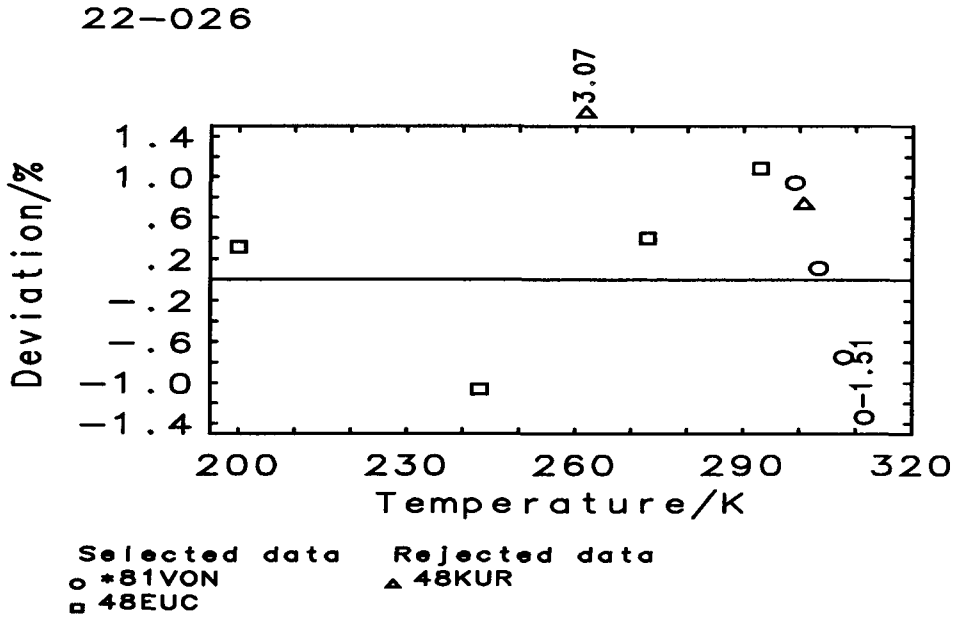
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	8	0.644	1.74–1	1.12	–9.04–3	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
200.0–311.6		1.61110+1	–4.40676	1.43637			V

TABLE 22.26.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J\,K^{-1}g^{-1}$)	1.38	1.40	1.42	1.44	1.46	1.49	1.52
C_p ($J\,K^{-1}mol^{-1}$)	108	110	111	113	115	117	119
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.55	1.57	1.59	1.63	1.67	1.67	1.72
C_p ($J\,K^{-1}mol^{-1}$)	122	123	125	128	131	132	135

TABLE 22.26.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	8	0.814	1.89–1	1.30	–1.35–2	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.0–311.6	503.00	–3.40854	1.24416	8.24083	2.33452		V



Name: 2–Chloro–1,3–butadiene
Formula: C_4H_5Cl

CAS–RN: 126–99–8
Group No.: 22–027
Molar Mass: 88.54

TABLE 22.27.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60JOH	N	293.15	1.314	nosp	not specified		C_p	not specified	

60JOH the origin of data is unclear

Name: 1,4–Dichlorobutane
Formula: $C_4H_8Cl_2$

CAS–RN: 110–56–5
Group No.: 22–028
Molar Mass: 127.01

TABLE 22.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85LAI/WIL	298.1	1	0.30	99.5	estim	C_p	FSIT	71PIC/LED
93HAL	298.1	1	0.15	99.9	chrom	C_p	DDCT	74SUU/WAD

TABLE 22.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
85LAI/WIL	298.1	1	0.30	0.595	3.94–2	0.18	–3.94–2	–1
93HAL	298.1	1	0.15	0.298	9.90–3	0.04	9.90–3	1

TABLE 22.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.665	4.06–2	0.18	–1.48–2	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		2.21201+1					III

TABLE 22.28.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1} g^{-1}$)	1.448
C_p ($J K^{-1} mol^{-1}$)	183.9

Name: 1–Chlorobutane
Formula: C_4H_9Cl

CAS–RN: 109–69–3
Group No.: 22–029
Molar Mass: 92.57

TABLE 22.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61ROU	300.9–309.0	12	nosp	not specified		C_p	BSAO	61ROU
85LAI/WIL	298.1	1	0.30	99.5	estim	C_p	FSIT	71PIC/LED

TABLE 22.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
61ROU	300.9–309.0	12	1.00#	0.597	1.17–1	0.60	3.64–2	2
85LAI/WIL	298.1	1	0.30	0.655	3.77–2	0.20	–3.77–2	–1

TABLE 22.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	13	13	0.654	1.23–1	0.63	3.07–2	1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–309.0		1.23357	6.03867				IV

TABLE 22.29.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p ($J K^{-1} g^{-1}$)	1.738	1.792
C_p ($J K^{-1} mol^{-1}$)	160.9	165.9

Name: 1–Chloro–2–methylpropane
Formula: C_4H_9Cl

CAS–RN: 513–36–0
Group No.: 22–030
Molar Mass: 92.57

TABLE 22.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	292.1–309.6	2	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 22.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	–3.82–6	0

Temp. range K	A_1	A_2	Level of uncertainty
292.1–309.6	–3.40121+1	1.72752+1	VI

able 22.30.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c ($J\,K^{-1}g^{-1}$)	1.44	1.57	1.60	1.76
C ($J\,K^{-1}mol^{-1}$)	134	145	148	162

Name: 2–Chloro–2–methylpropane
Formula: C_4H_9Cl

CAS–RN: 507–20–0
Group No.: 22–031
Molar Mass: 92.57

TABLE 22.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50KUS/CRO	251.6–259.6	4	2.00	not specified		C_p	BDHO	50KUS/CRO
66DWO/GUI	252.4–272.7	8	2.00	99.75	melpt	C_p	BSAO	66DWO/GUI
92KAL/KOH	293.1–313.1	2	1.00	98.8	chrom	C_p	FSIT	71PIC/LED

TABLE 22.31.2. Correlated heat capacities

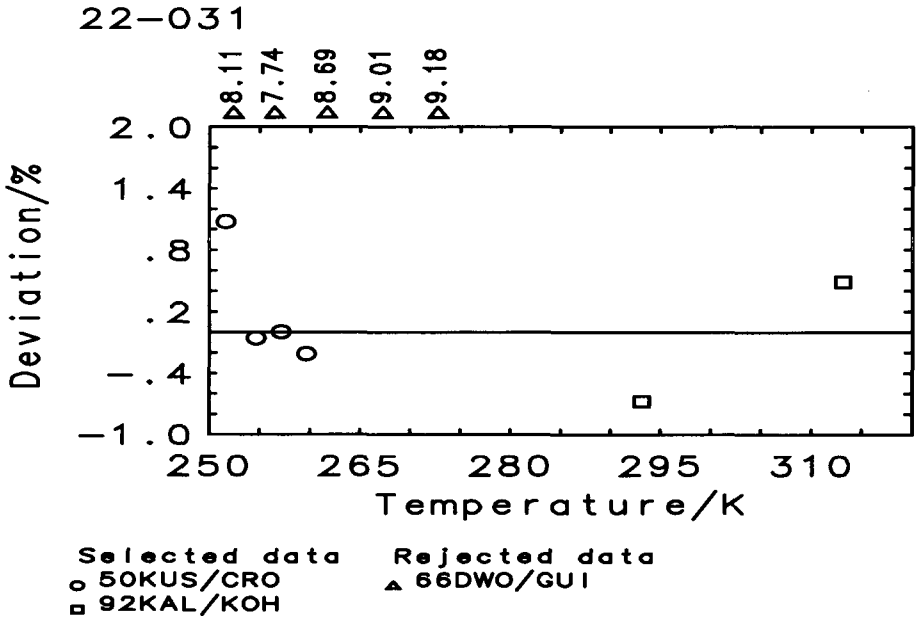
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50KUS/CRO	251.6–259.6	4	2.00	0.274	1.01–1	0.55	3.64–2	–1
92KAL/KOH	293.1–313.1	2	1.00	0.589	1.17–1	0.59	–1.61–2	0
				Rejected data				
66DWO/GUI	(1.84, 9.00, 1.83, 8)							

TABLE 22.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	6	0.499	1.30–1	0.69	1.89–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
251.6–313.1		9.10350	3.58306				V

TABLE 22.31.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	1.62	1.65	1.69	1.70	1.72	1.75	1.78
C_p ($J K^{-1} mol^{-1}$)	150	153	156	157	159	162	165
Temp. (K)	300	310					
c_p ($J K^{-1} g^{-1}$)	1.78	1.82					
C_p ($J K^{-1} mol^{-1}$)	165	168					



Name: 1,3–Dichloro–2,2–bis(chloromethyl)propane
Formula: $C_5H_8Cl_4$

CAS–RN: 3228–99–7
Group No.: 22–032
Molar Mass: 209.93

TABLE 22.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
65CLE/WON	372.8–397.6	8	0.15	99.07	melpt	C_{sat}	BSAO	53WES/HAT

TABLE 22.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.614	3.08–2	0.09	4.20–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
372.8–397.6		1.88473+1	3.81495				III

TABLE 22.32.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400
c_{sat} ($J\,K^{-1}g^{-1}$)	1.306	1.321	1.336	1.351
C_{sat} ($J\,K^{-1}mol^{-1}$)	274.1	277.2	280.4	283.6

Name: 1,5–Dichloropentane
Formula: $C_5H_{10}Cl_2$

CAS–RN: 628–76–2
Group No.: 22–033
Molar Mass: 141.04

TABLE 22.33.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
93HAL	298.15	1.513	0.15	99.9	chrom	C_p	DDCT	74SUU/WAD

Name: 1–Chloro–3–methylbutane
Formula: $C_5H_{11}Cl$

CAS–RN: 107–84–6
Group No.: 22–034
Molar Mass: 106.60

TABLE 22.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48KUR	307.3–329.1	2	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 22.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
307.3–329.1		1.16622+1	3.18413				VI

TABLE 22.34.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	1.68	1.70	1.73
C ($J\,K^{-1}mol^{-1}$)	179	182	184

Name: 1,2,4–Trichlorobenzene
Formula: $C_6H_3Cl_3$

CAS–RN: 120–82–1
Group No.: 22–035
Molar Mass: 181.45

TABLE 22.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
69WIL/ROT	293.1–303.1	2	0.40	not specified	C_p	BDAO	65FIN/GRU
74PET/TER	298.0–469.2	15	nosp	98. melpt	C_p	BDCT	74PET/TER
82WIL/ING	298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
86WIL/LAI	298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED

TABLE 22.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69WIL/ROT	293.1–303.1	2	0.40	3.229	2.95–1	1.29	–2.94–1	–2
74PET/TER	298.0–459.2	13	3.00#	0.750	5.69–1	2.25	1.68–2	1
82WIL/ING	298.1	1	0.30	3.491	2.45–1	1.05	2.45–1	1
86WIL/LAI	298.1	1	0.50#	2.450	2.87–1	1.23	2.87–1	1

TABLE 22.35.3. Parameters of regression polynomial

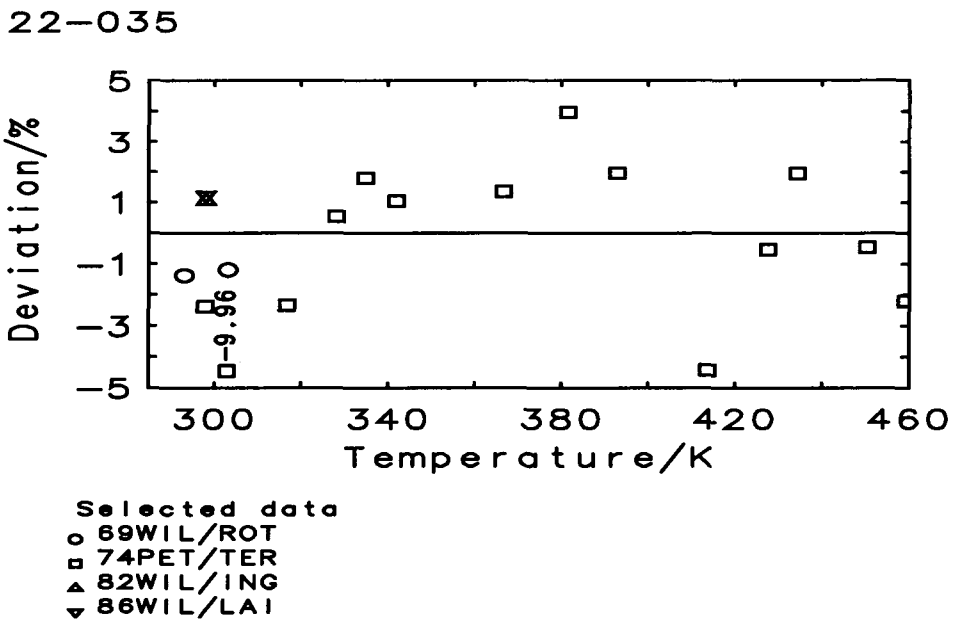
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	17	1.758	5.49–1	2.19	9.55–3	1
Temp. range K		A_1	A_2				Level of uncertainty
293.1–459.2		1.54985+1	2.56761				V

TABLE 22.35.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.05	1.06	1.06	1.07	1.09	1.10	1.11
C_p (J K^{-1}mol^{-1})	191	193	193	195	197	199	201
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	1.12	1.13	1.15	1.16	1.17	1.18	1.19
C_p (J K^{-1}mol^{-1})	204	206	208	210	212	214	216
Temp. (K)	420	430	440	450	460		
c_p (J K^{-1}g^{-1})	1.20	1.22	1.23	1.24	1.25		
C_p (J K^{-1}mol^{-1})	219	221	223	225	227		

TABLE 22.35.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	17	2.825	5.22–1	2.11	1.42–2	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
293.1–459.2	734.90	8.91423+1	1.37867+1	–1.24739+1	1.44094+2		V



Name: 1,2–Dichlorobenzene
Formula: $C_6H_4Cl_2$

CAS–RN: 95–50–1
Group No.: 22–036
Molar Mass: 147.00

TABLE 22.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	291.1–326.1	4S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 22.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/−
C	4	4	0.081	8.38–2	0.40	3.45–4	0
Temp. range K		A_1	A_2				Level of uncertainty
291.1–326.1		1.32591+1	2.42863				VI

TABLE 22.36.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c ($J K^{-1}g^{-1}$)	1.15	1.16	1.16	1.18	1.19	1.20
C ($J K^{-1}mol^{-1}$)	169	170	171	173	175	177

Name: 1,3–Dichlorobenzene
Formula: $C_6H_4Cl_2$

CAS–RN: 541–73–1
Group No.: 22–037
Molar Mass: 147.00

TABLE 22.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	253.9–327.5	6S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 22.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.071	7.38–2	0.36	3.82–4	–2

Temp. range K	A_1	A_2	Level of uncertainty
253.9–327.5	1.40629+1	2.17998	VI

TABLE 22.37.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c ($J K^{-1}g^{-1}$)	1.12	1.13	1.13	1.14	1.15	1.16	1.17
C ($J K^{-1}mol^{-1}$)	164	166	166	168	169	171	171

Temp. (K)	310	320	330
c ($J K^{-1}g^{-1}$)	1.18	1.19	1.20
C ($J K^{-1}mol^{-1}$)	173	175	177

Name: 1,4–Dichlorobenzene
Formula: $C_6H_4Cl_2$

CAS–RN: 106–46–7
Group No.: 22–038
Molar Mass: 147.00

TABLE 22.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	N	349.1	1	nosp	not specified		C_{avg}	DSIO	18NAR
76DWO/FIG		328.2–329.3	2	nosp	99.93	melpt	C_{sat}	BSAO	76DWO/FIG

18NAR average value in temperature range 326–372 K

TABLE 22.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
18NAR	349.1	1	5.00#	0.043	4.73–2	0.21	–4.73–2	–1
76DWO/FIG	328.2–329.3	2	2.00#	0.316	1.38–1	0.63	5.55–3	0

TABLE 22.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	3	3	0.449	2.01–1	0.92	−1.21–2	−1
Temp. range K		A_1	A_2				Level of uncertainty
328.2–349.1		1.75778+1	1.29282				VI

TABLE 22.38.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.24	1.24	1.25
C_{sat} (J K^{-1}mol^{-1})	182	183	184

Name: Chlorobenzene
Formula: C_6H_5Cl

CAS–RN: 108–90–7
Group No.: 22–039
Molar Mass: 112.56

TABLE 22.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		343.8–355.3	3S	nosp	not specified		C_{avg}	DSIO	*81VON
*87SCH		308.6–332.9	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
25WIL/DAN	N	293.1–353.1	4S	nosp	not specified		C_p	BSAO	24WIL/DAN
37STU		230.0–320.0	10S	nosp	not specified		C_p	BDHO	37STU
39PHI		305.5	1	nosp	not specified		C_p	BSIO	49WEI
49TSC/RIC3		298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
61ROU	N	296.1–318.1	2	nosp	not specified		C_p	BSAO	61ROU
71DES/BHA		298.1–318.1	3S	nosp	not specified		C_p	BSIO	56MUR/VAN
77FOR/BEN		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
88PER/AIC		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
90RAO/RAJ		318.1–333.1	4	4.00	not specified		C_p	BDHT	89PRA/RAJ
91TAN/ADA		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
92KAL/KOH		293.1–313.1	2	1.00	99.98	chrom	C_p	FSIT	71PIC/LED

25WIL/DAN origin of data unclear
61ROU constant value in temperature range 296–318 K obtained by the author

TABLE 22.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	343.8–355.3	3	2.00#	0.282	1.10–1	0.56	8.73–2	1
37STU	230.0–320.0	10	1.50#	0.836	2.18–1	1.25	2.36–2	2
77FOR/BEN	298.1	1	0.50#	0.215	1.94–2	0.11	–1.94–2	–1
91TAN/ADA	298.1	1	0.50#	0.264	2.39–2	0.13	–2.39–2	–1
92KAL/KOH	293.1–313.1	2	1.00	1.127	2.07–1	1.13	1.91–2	0
				Rejected data				
*87SCH	(3.10–1, 1.60, 2.59–1, 6)			25WIL/DAN	(4.83–1, 2.69, –4.49–1, –4)			
39PHI	(6.04–1, 3.19, 6.04–1, 1)			49TSC/RIC3	(5.93–1, 3.16, 5.93–1, 1)			
61ROU	(2.87–1, 1.55, 1.56–1, 0)			71DES/BHA	(3.04–1, 1.70, –2.91–1, –3)			
88PER/AIC	(3.40–1, 1.84, 3.40–1, 1)			90RAO/RAJ	(9.25–1, 4.67, 8.98–1, 4)			

TABLE 22.39.3. Parameters of regression polynomial

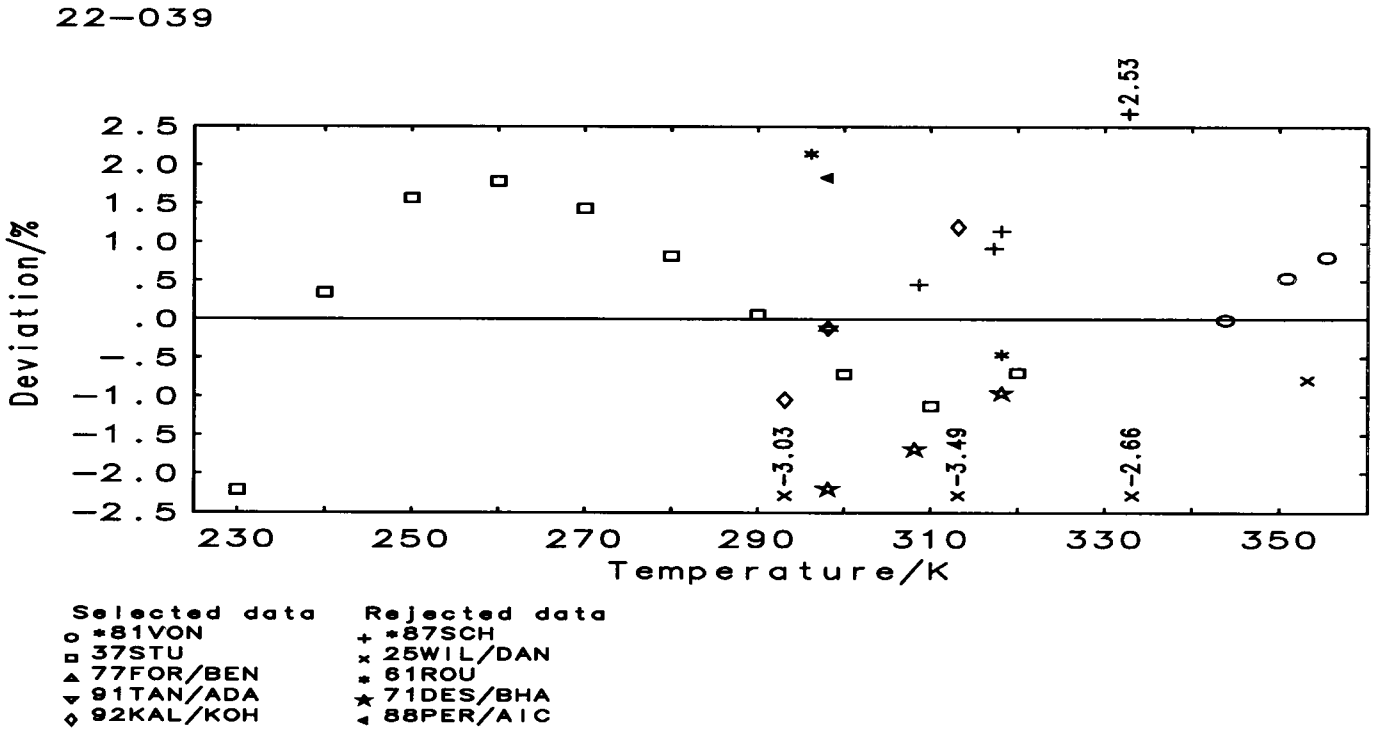
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	17	0.840	2.07–1	1.17	2.90–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
230.0–355.3		1.52484+1	–1.73449–1	3.85133–1			V

TABLE 22.39.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.25	1.26	1.27	1.29	1.30	1.30	1.31
C_p (J K^{-1}mol^{-1})	140	142	143	145	146	147	148
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.33	1.34	1.34	1.36	1.38	1.39	1.41
C_p (J K^{-1}mol^{-1})	150	151	151	153	155	157	159
Temp. (K)	350	360					
c_p (J K^{-1}g^{-1})	1.43	1.45					
C_p (J K^{-1}mol^{-1})	161	163					

TABLE 22.39.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	17	0.936	2.21–1	1.29	4.93–3	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
230.0–355.3	632.40	1.30912+1	8.99227	7.18891	4.76461		V



Name: 1,6–Dichlorohexane
Formula: $C_6H_{12}Cl_2$

CAS–RN: 2163–00–0
Group No.: 22–040
Molar Mass: 155.07

TABLE 22.40.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85LAI/GRO	298.15	1.545	nosp	not specified		C_p	FSIT	71PIC/LED

Name: (Chloromethyl)benzene
Formula: C_7H_7Cl

CAS–RN: 100–44–7
Group No.: 22–041
Molar Mass: 126.59

TABLE 22.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	317.5–346.5	6S	nosp	not specified		C_p	DSIO	*86SCH
31SMI/AND1	246.0–298.5	5	nosp	99.5	estim	C_p	DSIO	26AND/LYN

TABLE 22.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*87SCH	317.5–346.5	6	2.00#	0.061	2.82–2	0.12	1.88–3	1
31SMI/AND1	246.0–298.5	5	1.50#	0.205	6.58–2	0.31	–7.87–4	1

TABLE 22.41.3. Parameters of regression polynomial

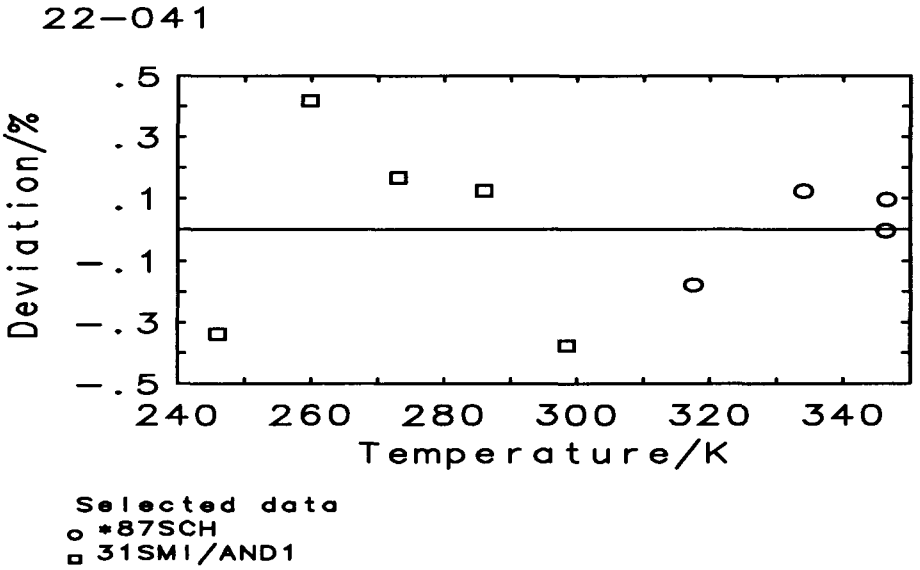
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.171	5.75–2	0.27	6.69–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
246.0–346.5		2.95624+1	–8.17737	1.89337			V

TABLE 22.41.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	1.38	1.39	1.40	1.40	1.41	1.43	1.45
C_p ($J K^{-1} mol^{-1}$)	174	175	177	178	179	181	183
Temp. (K)	300	310	320	330	340	350	
c_p ($J K^{-1} g^{-1}$)	1.45	1.47	1.50	1.52	1.55	1.59	
C_p ($J K^{-1} mol^{-1}$)	184	186	189	193	197	201	

TABLE 22.41.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.147	5.05–2	0.23	–3.45–3	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
246.0–346.5	660.00	6.04442+1	2.98666+1	–9.94535	3.05818+1		V



Name: 1–Chloro–2–methylbenzene
Formula: C_7H_7Cl

CAS–RN: 95–49–8
Group No.: 22–042
Molar Mass: 126.59

TABLE 22.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	N	316.6–345.8	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

*87SCH unspecified isomer; probably 1-Chloro-2-methylbenzene (according to n.b.t.)

TABLE 22.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.024	1.09–2	0.05	3.82–6	–2
Temp. range K		A_1	A_2				Level of uncertainty
316.6–345.8		7.02596	4.78215				V

TABLE 22.42.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J K^{-1}g^{-1}$)	1.47	1.50	1.53	1.56
C ($J K^{-1}mol^{-1}$)	186	190	194	198

Name: 3–Chloroheptane
Formula: $C_7H_{15}Cl$

CAS–RN: 999–52–0
Group No.: 22–043
Molar Mass: 134.65

TABLE 22.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88MEL/VER	233.1–573.2	11	2.50	not specified		C_{sat}	not specified	

TABLE 22.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.443	6.05–1	1.11	6.58–3	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
233.1–573.2		1.29397+1	1.22924+1	–3.56564	5.18093–1		V

TABLE 22.43.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.77	1.79	1.82	1.85	1.87	1.88	1.90
C_{sat} (J K^{-1}mol^{-1})	238	242	245	249	252	253	256
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.93	1.95	1.96	1.99	2.02	2.06	2.09
C_{sat} (J K^{-1}mol^{-1})	260	263	264	268	272	277	282
Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	2.13	2.17	2.21	2.26	2.31	2.36	2.41
C_{sat} (J K^{-1}mol^{-1})	287	292	298	304	311	318	325
Temp. (K)	420	430	440	450	460	470	480
c_{sat} (J K^{-1}g^{-1})	2.47	2.54	2.60	2.67	2.75	2.82	2.91
C_{sat} (J K^{-1}mol^{-1})	333	341	350	360	370	380	392
Temp. (K)	490	500	510	520	530	540	550
c_{sat} (J K^{-1}g^{-1})	3.00	3.09	3.19	3.29	3.40	3.52	3.64
C_{sat} (J K^{-1}mol^{-1})	403	416	429	443	458	473	490
Temp. (K)	560	570					
c_{sat} (J K^{-1}g^{-1})	3.76	3.90					
C_{sat} (J K^{-1}mol^{-1})	507	525					

Name: 1-Chloronaphthalene
Formula: $C_{10}H_7Cl$

CAS-RN: 90-13-1
Group No.: 22-044
Molar Mass: 162.62

TABLE 22.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81GRO/ING	298.1	1	nosp	99.0	chrom	C_p	FSIT	71PIC/LED
86WIL/LAI	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
88COS/VAN	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 22.44.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
81GRO/ING	298.1	1	0.50#	0.043	5.42-3	0.02	5.42-3	1
86WIL/LAI	298.1	1	0.50#	0.043	5.41-3	0.02	-5.41-3	-1
				Rejected data				
88COS/VAN	(1.53-1, 0.60, 1.53-1, 1)							

TABLE 22.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	2	0.060	7.65–3	0.03	2.86–6	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		2.54164+1					III

TABLE 22.44.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1}g^{-1}$)	1.300
C_p ($J K^{-1}mol^{-1}$)	211.3

Name: 2–Chloronaphthalene
Formula: $C_{10}H_7Cl$

CAS–RN: 91–58–7
Group No.: 22–045
Molar Mass: 162.62

TABLE 22.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91VAN/VER	333.5–367.5	34	nosp	99.91	melpt	C_p	BSAO	87VAN/VAN

TABLE 22.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.204	1.69–2	0.06	2.02–5	11
Temp. range K		A_1	A_2				Level of uncertainty
333.5–367.5		1.19413+1	4.58432				III

TABLE 22.45.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	1.407	1.431	1.454	1.478
C_p ($J K^{-1}mol^{-1}$)	228.9	232.7	236.5	240.3

Name: 2–Chloro–1,1'–biphenyl
Formula: $C_{12}H_9Cl$

CAS–RN: 2051–60–7
Group No.: 22–046
Molar Mass: 188.66

TABLE 22.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74GEI/DZH2	304.8–330.0	4S	nosp	99.66	melpt	C_p	BSAO	54STR/ICK

TABLE 22.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.006	1.78–3	0.01	–4.77–7	0
Temp. range K		A_1	A_2				Level of uncertainty
304.8–330.0		1.80393+1	4.46051				IV

TABLE 22.46.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.404	1.424	1.444
C_p ($J\,K^{-1}mol^{-1}$)	265.0	268.7	272.4

Name: 4–Chloro–1,1'–biphenyl
Formula: $C_{12}H_9Cl$

CAS–RN: 2051–62–9
Group No.: 22–047
Molar Mass: 188.66

TABLE 22.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75GEI/DZH	347.9–370.0	2S	0.30	99.1	melpt	C_p	BSAO	54STR/ICK

TABLE 22.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
347.9–370.0		2.48100+1	2.28571				IV

TABLE 22.47.4. Recommended values of heat capacities

Temp. (K)	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	1.446	1.456	1.466
C_p ($J\,K^{-1}mol^{-1}$)	272.8	274.7	276.6

Name: 1,1'–(Chloromethylene)bisbenzene
Formula: $C_{13}H_{11}Cl$

CAS–RN: 90–99–3
Group No.: 22–048
Molar Mass: 202.68

TABLE 22.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31SMI/AND1	298.5–310.7	2	nosp	98.5	estim	C_p	DSIO	26AND/LYN

TABLE 22.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.5–310.7	1.89174+1	5.36208	V

TABLE 22.48.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.44	1.46
C_p ($J\,K^{-1}mol^{-1}$)	291	295

Name: 1–Chlorooctadecane
Formula: $C_{18}H_{37}Cl$

CAS–RN: 3386–33–2
Group No.: 22–049
Molar Mass: 288.94

TABLE 22.49.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75STR/SUN	N	301.00	2.100	3.00		not specified	C_p	BDHT	69PER/COM

75STR/SUN content of Octadecane below 0.02 mass %

23. Bromine Derivatives

The bromine family contains 40 compounds, of which 8 were measured only at one temperature.

Some laboratories produced values for a large number of bromine derivatives but in most cases the data pertain to the older literature (such as measurements from THA, *81VON) and/or sources reporting poor quality data (such as results for 14 compounds from PTIL, 48KUR). These sources had to be included only because of the absence of better quality data or for extending data over a temperature interval. The remaining articles containing more than one measured bromine compound are those from JHUB (31DEE) and from PUP (50KUS/CRO, 50CRO/SMI2); the uncertainty of these measurements is according to our judgement between 1.5 to 2 %.

With some exceptions, only data for bromoalkanes were reported. Measurements over a wide temperature range were performed for bromomethane at UCB (38EGA/KEM) and for dibromomethane at UCE (57HAR/MOE). The most frequently measured compound in the bromine family is 1,2-dibromoethane, but most of the data are from older sources. Since the two more reliable measurements from UCB (40PIT1) and UWA (69WIL/SCH) were carried out over a narrow temperature interval, some of the less reliable measurements had to be taken account (33LEB/MOE, 39RAI) in the correlation to obtain the recommended values. The data measured for 3-bromohexane at KGPI (88MEL/VER) gave results with a reported error of 2.5 %, and those for 1-bromodocosane and 1-bromotriacontane from General Electric Research Laboratory Schenectady, N.Y. (53HOF/DEC) seem also to be of poor quality with a reported error of 4 % for sample purity of only 90 %.

The most accurate measurements in this family appear to be the data for bromobenzene from NBSW (75MAS/SCO) and those for pentaerythrityl bromide from UMAA (65CLE/WON). The former data have been supplemented by the older measurements of (*81VON).

Unusual studies were carried out on 10 brominated and deuterated ethanes at one temperature in Belgium (49WUY/JUN, 49DHO/JUN). As for some of these compounds, any new information has not been published since this time, hence, their CASRN's are not assigned or available.

Name: Tetrabromomethane
Formula: CBr_4

CAS-RN: 558-13-4
Group No.: 23-001
Molar Mass: 331.63

TABLE 23.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
39FRE/HIL	N	363.3–423.1	2	nosp	not specified	C_{avg}	DSIO	38FRE/HIL1
48KUR		403.9–446.8	3	nosp	not specified	C_{avg}	DSIO	47KUR

39FRE/HIL constant value calculated from temperature dependence of enthalpy by authors

TABLE 23.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
39FRE/HIL	363.3	1	3.00#	0.154	8.56–2	0.46	–8.56–2	–1
48KUR	403.9–446.8	3	5.00#	0.323	3.41–1	1.61	8.94–2	1

TABLE 23.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	4	0.410	4.22–1	2.00	4.57–2	0
Temp. range K		A_1	A_2				Level of uncertainty
363.3–446.8		2.77717	4.34315				VI

TABLE 23.1.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c ($J K^{-1} g^{-1}$)	0.46	0.47	.48	0.49	0.51	0.52	0.53
C ($J K^{-1} mol^{-1}$)	153	157	160	164	168	171	175
Temp. (K)	430	440	450				
c ($J K^{-1} g^{-1}$)	0.54	0.55	0.56				
C ($J K^{-1} mol^{-1}$)	178	182	186				

Name: Tribromomethane
Formula: $CHBr_3$

CAS–RN: 75–25–2
Group No.: 23–002
Molar Mass: 252.73

TABLE 23.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
22COH/MOE	292.1–292.1	2	nosp	not	specified	C_p	BSAO	20COH/MOE
32TRE	298.0	1	nosp	not	specified	C_p	BSIO	49WEI
48KUR	305.2–356.9	4	nosp	not	specified	C_{avg}	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not	specified	C_p	BSIO	49TSC/RIC1

TABLE 23.2.2. Correlated heat capacities

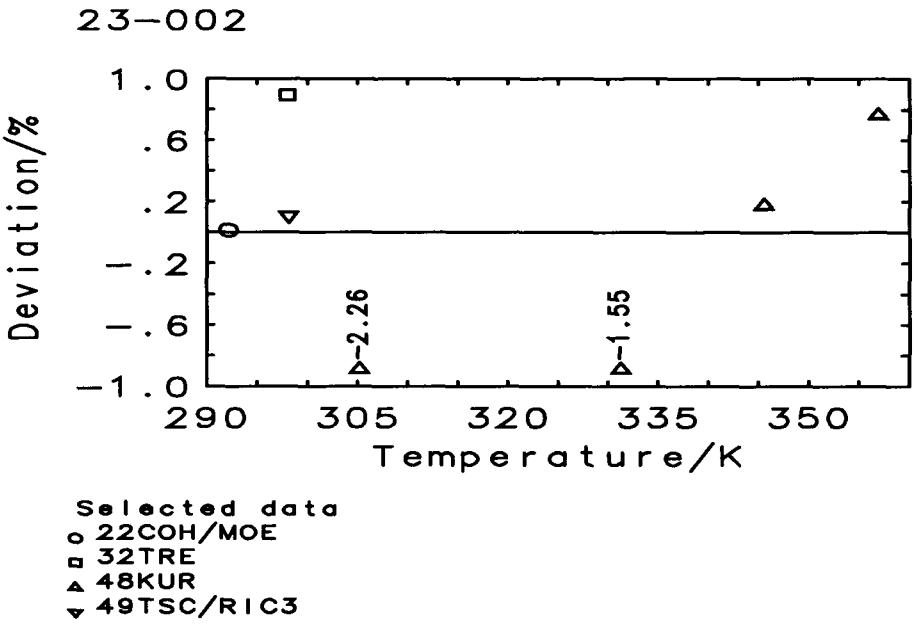
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
22COH/MOE	292.1	2	0.70#	0.069	7.80–3	0.05	–4.51–3	0
32TRE	298.0	1	2.00#	0.447	1.45–1	0.89	1.45–1	1
48KUR	305.2–356.9	4	5.00#	0.285	2.28–1	1.43	–1.13–1	0
49TSC/RIC3	298.1	1	3.00#	0.035	1.70–2	0.11	1.70–2	1

TABLE 23.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.299	1.96–1	1.22	–3.74–2	2
Temp. range K		A_1	A_2				Level of uncertainty
292.1–356.9		1.37276+1	8.07330–1				VI

TABLE 23.2.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	0.53	0.53	0.53	0.53	0.54	0.54	0.54
C_p ($J K^{-1} mol^{-1}$)	134	134	134	135	136	136	137
Temp. (K)	350	360					
c_p ($J K^{-1} g^{-1}$)	0.54	0.55					
C_p ($J K^{-1} mol^{-1}$)	138	138					



Name: Dibromomethane
Formula: CH_2Br_2

CAS–RN: 74–95–3
Group No.: 23–003
Molar Mass: 173.83

TABLE 23.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
48KUR	272.1–329.9	4	nosp	not specified	C_{avg}	DSIO	47KUR
57HAR/MOE	244.9–303.2	7	0.50	not specified	C_p	BSIO	57HAR/MOE

TABLE 23.3.2. Correlated heat capacities

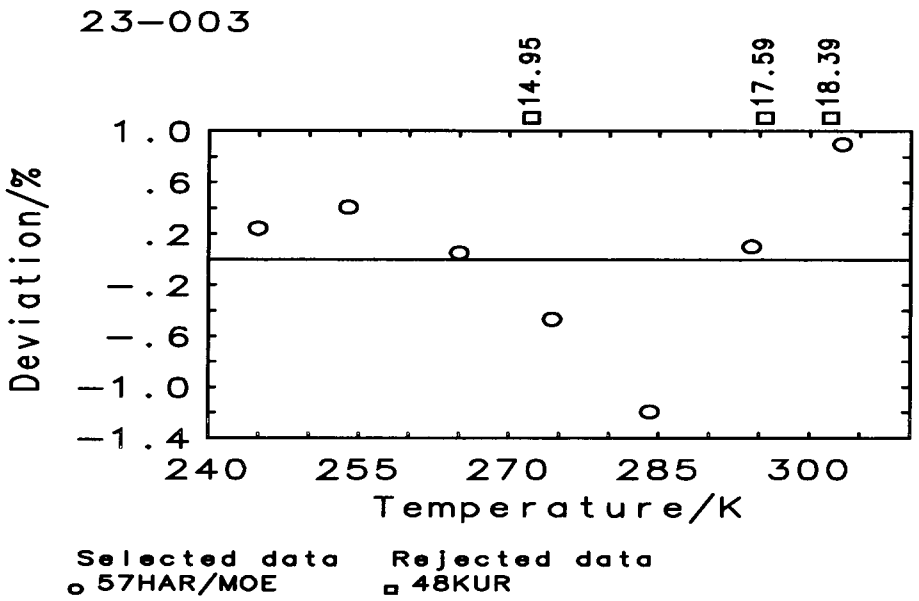
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57HAR/MOE	244.9–303.2	7	0.50	1.241	7.77–2	0.62	9.66–4	3
				Rejected data				
48KUR	(2.59, 17.04, 2.58, 3)							

TABLE 23.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	7	1.468	9.19–2	0.73	9.66–4	3
Temp. range K		A_1	A_2				Level of uncertainty
244.9–303.2		1.25861+1	−4.53477–3				IV

TABLE 23.3.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	0.601	0.601	0.601	0.601	0.601	0.601	0.601
C_p ($J K^{-1} mol^{-1}$)	104.6	104.6	104.5	104.5	104.5	104.5	104.5
Temp. (K)	298.15	300					
c_p ($J K^{-1} g^{-1}$)	0.601	0.601					
C_p ($J K^{-1} mol^{-1}$)	104.5	104.5					



Name: Bromomethane
Formula: CH_3Br

CAS–RN: 74–83–9
Group No.: 23–004
Molar Mass: 94.94

TABLE 23.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38EGA/KEM		184.5–275.6	16	nosp	99.999	melpt	C_p	BSIO	28GIA/WIE1
48KUR	N	244.1–266.5	3	nosp	not specified		C_{avg}	DSIO	47KUR

48KUR suspect values

TABLE 23.4.2. Correlated heat capacities

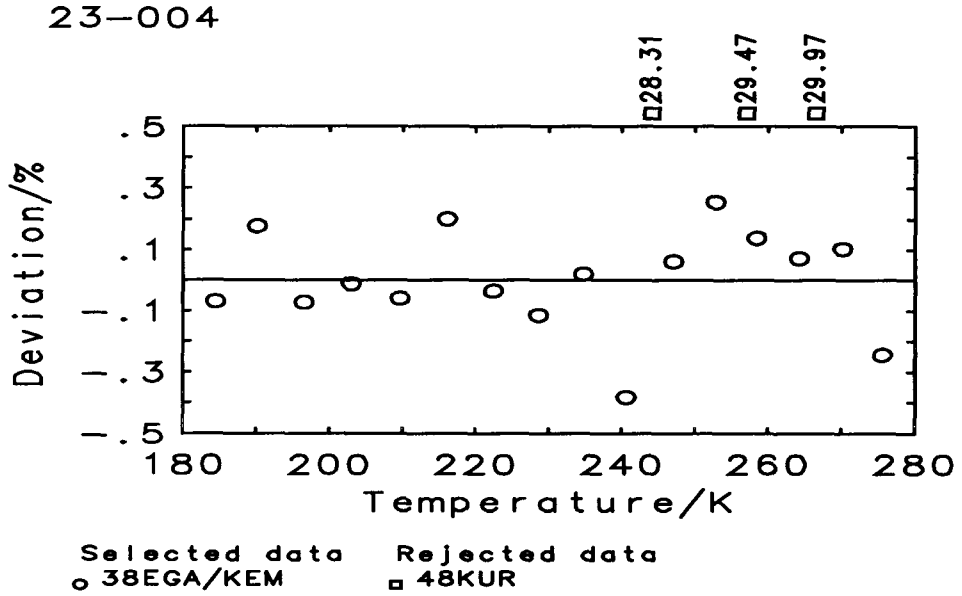
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
38EGA/KEM	184.5–275.6	16	0.30#	0.534	1.50–2	0.16	4.79–5	0
				Rejected data				
48KUR	(3.87, 29.26, 3.87, 3)							

TABLE 23.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	16	0.593	1.66–2	0.18	4.79–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
184.5–275.6		1.27783+1	–3.14160	7.04852–1			III

TABLE 23.4.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	0.819	0.816	0.814	0.813	0.813	0.814	0.817
C_p (J K^{-1}mol^{-1})	77.77	77.45	77.24	77.14	77.17	77.31	77.57
Temp. (K)	260	270					
c_p (J K^{-1}g^{-1})	0.821	0.826					
C_p (J K^{-1}mol^{-1})	77.95	78.44					



Name: 1,2–Dibromoethane–1,1,2,2–d_4
Formula: $C_2Br_2D_4$

CAS–RN: 22581–63–1
Group No.: 23–005
Molar Mass: 191.89

TABLE 23.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49DHO/JUN	N	293.1	1	nosp	not specified		C_p	BDHO	49WUY/JUN
49WUY/JUN	N	310.1	1	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (3.5 % of isotope D_3H)
49WUY/JUN correction for incomplete deuteration (3.5 % of isotope D_3H)

TABLE 23.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
49DHO/JUN	293.1	1	3.00#	0.000	0.00	0.00	0.00	0
49WUY/JUN	310.1	1	3.00#	0.000	0.00	0.00	0.00	0

TABLE 23.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–310.1		1.47018+1	1.04235				V

TABLE 23.5.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p (J K^{-1}g^{-1})	0.77	0.77	0.77	0.78
C_p (J K^{-1}mol^{-1})	147	148	148	149

Name: 1,1,2–Tribromoethane–1,2,2–d_3
Formula: $C_2Br_3D_3$

CAS–RN: unknown
Group No.: 23–006
Molar Mass: 269.78

TABLE 23.6.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49DHO/JUN	N	293.15	0.6627	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (1.0 % of isotope D_2H)

Name: 1,2–Dibromoethane–1,1,2–d_3
Formula: $C_2HBr_2D_3$

CAS–RN: 117164–17–7
Group No.: 23–007
Molar Mass: 190.88

TABLE 23.7.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49WUY/JUN	N	310.15	0.7604	nosp	not specified		C_p	BDHO	49WUY/JUN

49WUY/JUN correction for incomplete deuteration (7.0 % of isotope D_2H_2)

Name: 1,1,2–Tribromoethane–2,2–d_2
Formula: $C_2HBr_3D_2$

CAS–RN: unknown
Group No.: 23–008
Molar Mass: 268.77

TABLE 23.8.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49DHO/JUN	N	293.15	0.6489	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (6.0 % of isotope HDH)

Name: 1,2–Dibromoethane–1,1–d_2
Formula: $C_2H_2Br_2D_2$

CAS–RN: unknown
Group No.: 23–009
Molar Mass: 189.87

TABLE 23.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49DHO/JUN	N	293.1	1	nosp	not specified		C_p	BDHO	49WUY/JUN
49WUY/JUN	N	310.1	1	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (8.0 % of isotope H_3D)
49WUY/JUN correction for incomplete deuteration (8.0 % of isotope H_3D)

TABLE 23.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
49DHO/JUN	293.1	1	3.00#	0.000	0.00	0.00	0.00	0
49WUY/JUN	310.1	1	3.00#	0.000	0.00	0.00	0.00	0

TABLE 23.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–310.1		1.51763+1	6.76794–1				V

TABLE 23.9.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	0.75	0.75	0.75	0.76
C_p ($J\,K^{-1}mol^{-1}$)	143	143	143	144

Name: 1,2–Dibromoethane–1,2–d_2
Formula: $C_2H_2Br_2D_2$

CAS–RN: unknown
Group No.: 23–010
Molar Mass: 189.87

TABLE 23.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
49DHO/JUN	N	293.1	1	nosp	not specified	C_p	BDHO	49WUY/JUN
49WUY/JUN	N	310.1	1	nosp	not specified	C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (2.0 % of isotope H_3D)
49WUY/JUN correction for incomplete deuteration (2.0 % of isotope H_3D)

TABLE 23.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
49DHO/JUN	293.1	1	3.00#	0.000	0.00	0.00	0.00	0
49WUY/JUN	310.1	1	3.00#	0.000	0.00	0.00	0.00	0

TABLE 23.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–310.1		1.60341+1	3.41819–1				V

TABLE 23.10.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	0.75	0.75	0.75	0.75
C_p ($J K^{-1}mol^{-1}$)	142	142	142	142

Name: 1,1,2–Tribromoethane–1–*d*
Formula: $C_2H_2Br_3D$

CAS–RN: unknown
Group No.: 23–011
Molar Mass: 267.76

TABLE 23.11.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49DHO/JUN	N	293.15	0.6339	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (8.0 % of isotope H_3)

Name: 1,1,2–Tribromoethane–2–*d*
Formula: $C_2H_2Br_3D$

CAS–RN: unknown
Group No.: 23–012
Molar Mass: 267.76

TABLE 23.12.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49DHO/JUN	N	293.15	0.6326	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (3.0 % of isotope H_3)

Name: 1,1,2,2–Tetrabromoethane
Formula: $C_2H_2Br_4$

CAS–RN: 79–27–6
Group No.: 23–013
Molar Mass: 345.65

TABLE 23.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
48KUR	306.5–346.8	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 23.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.000	4.20–4	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
306.5–346.8		7.26458	4.24055				VI

TABLE 23.13.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c ($J K^{-1} g^{-1}$)	0.49	0.50	0.51	0.52	0.53
C ($J K^{-1} mol^{-1}$)	170	173	177	180	184

Name: Bromoethene
Formula: C_2H_3Br

CAS–RN: 593–60–2
Group No.: 23–014
Molar Mass: 106.95

TABLE 23.14.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34MEH2	288.15	1.004	1.50	not specified		C_p	BSIO	49WEI

Name: 1,2–Dibromoethane–*d*
Formula: $C_2H_3Br_2D$

CAS–RN: unknown
Group No.: 23–015
Molar Mass: 188.87

TABLE 23.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49DHO/JUN	N	293.1	1	nosp	not specified		C_p	BDHO	49WUY/JUN
49WUY/JUN	N	310.1	1	nosp	not specified		C_p	BDHO	49WUY/JUN

49DHO/JUN correction for incomplete deuteration (6.5 % of isotope H_4)
49WUY/JUN correction for incomplete deuteration (6.5 % of isotope H_4)

TABLE 23.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
49DHO/JUN	293.1	1	3.00#	0.000	0.00	0.00	0.00	0
49WUY/JUN	310.1	1	3.00#	0.000	0.00	0.00	0.00	0

TABLE 23.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
293.1–310.1	1.52613+1	4.41708–1	V

TABLE 23.15.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	0.73	0.73	0.73	0.73
C_p ($J\,K^{-1}mol^{-1}$)	138	138	138	138

Name: 1,1,2–Tribromoethane
Formula: $C_2H_3Br_3$

CAS–RN: 78–74–0
Group No.: 23–016
Molar Mass: 266.76

TABLE 23.16.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
49DHO/JUN	293.15	0.6209	nosp	not specified	C_p	BDHO	49WUY/JUN

Name: 1,2–Dibromoethane
Formula: $C_2H_4Br_2$

CAS–RN: 106–93–4
Group No.: 23–017
Molar Mass: 187.86

TABLE 23.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
33LEB/MOE		283.3–298.5	5	nosp	not specified	C_p	BSIO	33LEB/MOE
39RAI	N	283.3–321.7	9	2.00	99.92 melpt	C_p	BDHO	37STU
40PIT1		286.5–318.0	4	0.20	99.74 melpt	C_p	BSIO	28LAT/GRE
48KUR		309.1–345.7	3	nosp	not specified	C_{avg}	DSIO	47KUR
49DHO/JUN		293.1	1	nosp	not specified	C_p	BDHO	49WUY/JUN
49TSC/RIC3		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
49WUY/JUN		310.1	1	nosp	not specified	C_p	BDHO	49WUY/JUN
65FIN/GRU		300.0	1	0.40	not specified	C_p	BDAO	65FIN/GRU
69WIL/SCH		293.1–313.1	3	0.40	not specified	C_p	BDAO	65FIN/GRU

39RAI data from a graph only

TABLE 23.17.2. Correlated heat capacities

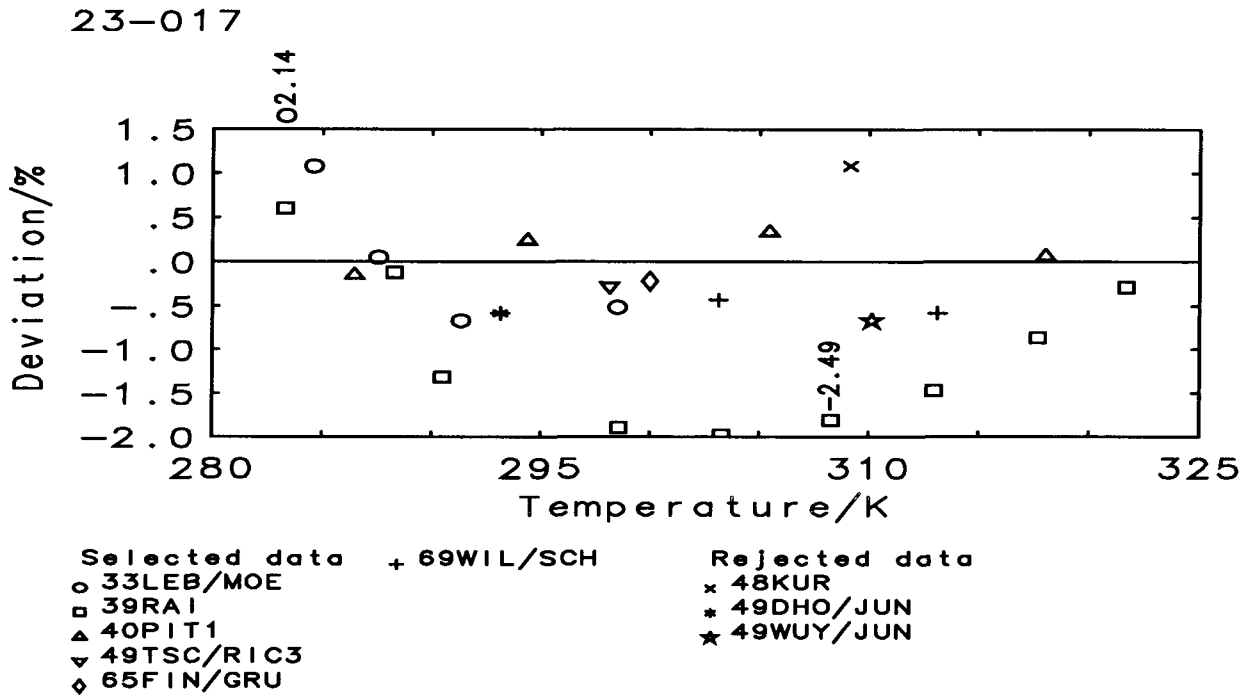
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33LEB/MOE	283.3–298.5	5	1.00#	1.137	1.89–1	1.14	7.02–2	1
39RAI	283.3–321.7	9	2.00	0.723	2.32–1	1.45	–1.75–1	–7
40PIT1	286.5–318.0	4	0.20	1.101	3.60–2	0.22	1.97–2	2
49TSC/RIC3	298.1	1	3.00#	0.093	4.55–2	0.28	–4.55–2	–1
65FIN/GRU	300.0	1	0.40	0.552	3.60–2	0.22	–3.60–2	–1
69WIL/SCH	293.1–313.1	3	0.40	1.346	8.75–2	0.54	–8.67–2	–3
				Rejected data				
48KUR	(1.79–1, 1.08, 1.79–1, 1)			49DHO/JUN	(9.48–2, 0.58, –9.48–2, –1)			
49WUY/JUN	(1.10–1, 0.67, –1.10–1, –1)							

TABLE 23.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	28	23	1.043	1.86–1	1.15	–6.47–2	–9
Temp. range K		A_1	A_2	A_3			Level of uncertainty
283.3–321.7		4.32852+1	–1.82118+1	3.07322			IV

TABLE 23.17.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	0.722	0.722	0.722	0.724	0.729
C_p (J K^{-1}mol^{-1})	135.7	135.6	135.6	136.0	137.0



Name: Bromoethane
Formula: C_2H_5Br

CAS–RN: 74–96–4
Group No.: 23–018
Molar Mass: 108.97

TABLE 23.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
07BAT	N	167.7–244.3	5	nosp	not specified		C_p	BSIO	07BAT
12SCH2		280.6–290.6	3	nosp	not specified		C_p	BSIO	12SCH1
48KUR		256.5–300.0	5	nosp	not specified		C_{avg}	DSIO	47KUR
49TSC/RIC3		298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1

07BAT same data in 08BAT

TABLE 23.18.2. Correlated heat capacities

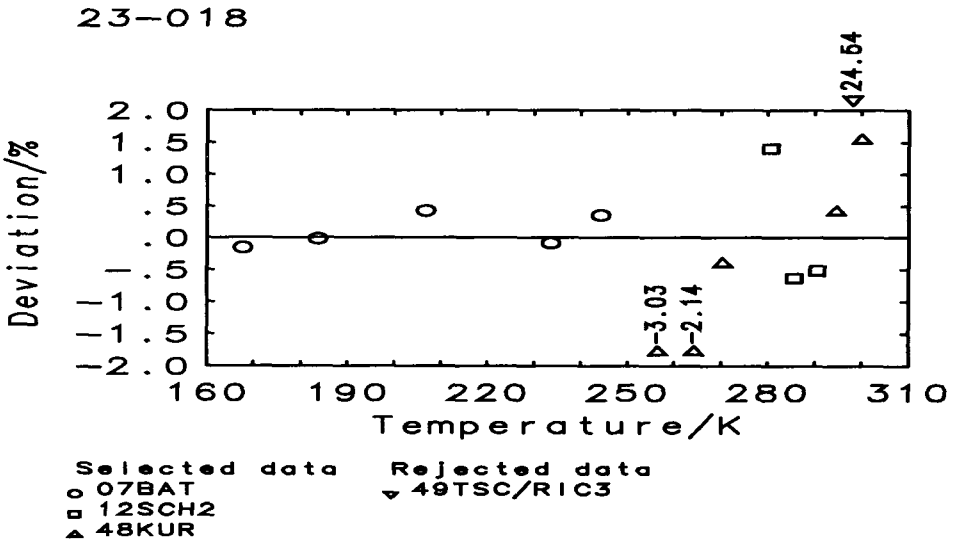
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
07BAT	167.7–244.3	5	2.00#	0.130	2.86–2	0.26	1.14–2	–1
12SCH2	280.6–290.6	3	3.00#	0.313	1.11–1	0.94	1.05–2	–1
48KUR	256.5–300.0	5	5.00#	0.363	2.04–1	1.81	–7.67–2	–1
				Rejected data				
49TSC/RIC3	(3.90, 24.54, 3.90, 1)							

TABLE 23.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	0.322	1.58–1	1.39	–2.27–2	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
167.7–300.0		1.22805+1	–2.02028	6.46068–1			VI

TABLE 23.18.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	0.82	0.82	0.82	0.83	0.83	0.84	0.84
C_p (J K^{-1}mol^{-1})	89.1	89.3	89.6	90.0	90.5	91.2	91.9
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	0.85	0.86	0.87	0.88	0.88	0.89	0.90
C_p (J K^{-1}mol^{-1})	92.7	93.7	94.7	95.9	96.3	97.2	98.6
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	0.92	0.92					
C_p (J K^{-1}mol^{-1})	99.8	100					



Name: 3–Bromo–1–propene
Formula: C_3H_5Br

CAS–RN: 106–95–6
Group No.: 23–019
Molar Mass: 120.98

TABLE 23.19.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49TSC/RIC3	298.15	1.088	nosp	not specified		C_p	BSIO	49TSC/RIC1

Name: 1,2,3–Tribromopropane
Formula: $C_3H_5Br_3$

CAS–RN: 96–11–7
Group No.: 23–020
Molar Mass: 280.78

TABLE 23.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	320.2–390.6	6	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 23.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.392	4.95–1	1.96	1.35–2	–2
Temp. range K		A_1	A_2				Level of uncertainty
320.2–390.6		4.78323	5.32870				VI

TABLE 23.20.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J\,K^{-1}g^{-1}$)	0.65	0.66	0.68	0.69	0.71	0.73	0.74
C ($J\,K^{-1}mol^{-1}$)	182	186	190	195	199	204	208
Temp. (K)	390						
c ($J\,K^{-1}g^{-1}$)	0.76						
C ($J\,K^{-1}mol^{-1}$)	213						

Name: 1,2–Dibromopropane
Formula: $C_3H_6Br_2$

CAS–RN: 78–75–1
Group No.: 23–021
Molar Mass: 201.89

TABLE 23.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	305.4–346.6	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 23.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.002	2.01–3	0.01	–6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
305.4–346.6		8.07941	3.74501				VI

TABLE 23.21.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c ($J K^{-1}g^{-1}$)	0.81	0.83	0.84	0.86	0.87
C ($J K^{-1}mol^{-1}$)	164	167	170	173	176

Name: 1,3–Dibromopropane
Formula: $C_3H_6Br_2$

CAS–RN: 109–64–8
Group No.: 23–022
Molar Mass: 201.89

TABLE 23.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	332.3–358.3	3	nosp	not specified		C_{avg}	DSIO	47KUR
50CRO/SMY2	243.1–245.6	2	1.40	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48KUR	332.3–358.4	3	5.00#	0.224	2.32–1	1.12	–1.69–2	–1
50CRO/SMY2	243.1–245.6	2	1.40	0.200	5.24–2	0.28	2.91–3	0

TABLE 23.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.277	2.36–1	1.14	–9.00–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
243.1–358.4		1.41627+1	1.85308				VI

TABLE 23.22.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	0.77	0.77	0.78	0.79	0.79	0.80	0.80
C_p ($J K^{-1}mol^{-1}$)	155	156	158	159	160	161	162
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	0.81	0.81	0.82	0.83	0.84	0.84	0.85
C_p ($J K^{-1}mol^{-1}$)	164	164	166	167	169	170	172
Temp. (K)	360						
c_p ($J K^{-1}g^{-1}$)	0.86						
C_p ($J K^{-1}mol^{-1}$)	173						

Name: 1-Bromopropane
Formula: C_3H_7Br

CAS-RN: 106-94-5
Group No.: 23-023
Molar Mass: 122.99

TABLE 23.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	305.1-323.3	3S	nosp	not	specified	C_{avg}	DSIO	*81VON
48KUR	268.1-312.9	3	nosp	not	specified	C_{avg}	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not	specified	C_p	BSIO	49TSC/RIC1

TABLE 23.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
*81VON	305.1-323.3	3	3.00#	0.585	2.79-1	1.75	-2.26-1	-3
48KUR	268.1-312.9	3	5.00#	0.791	6.78-1	3.96	4.46-1	1
49TSC/RIC3	298.1	1	3.00#	0.592	2.95-1	1.78	2.95-1	1

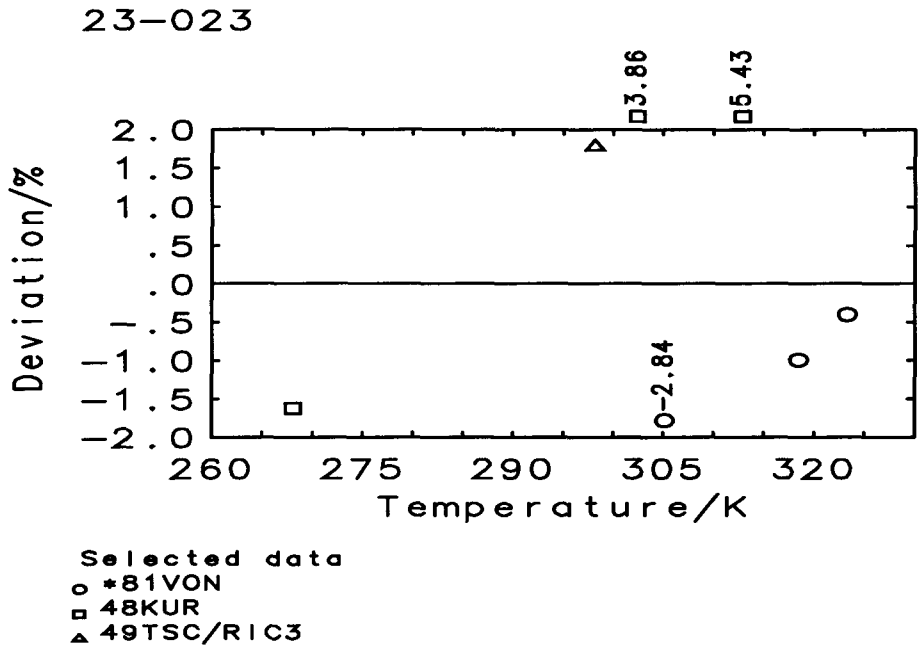
TABLE 23.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.807	5.83-1	3.45	1.36-1	-1
Temp. range K		A_1	A_2				Level of uncertainty
268.1-323.3		1.45860+1	5.72349-1				VI

TABLE 23.23.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	1.09	1.09	1.09	1.10	1.10	1.10	1.11
C_p ($J K^{-1} mol^{-1}$)	134	134	135	135	135	136	136

Temp. (K)	320
c_p ($J K^{-1} g^{-1}$)	1.11
C_p ($J K^{-1} mol^{-1}$)	137



Name: 2–Bromopropane
Formula: C_3H_7Br

CAS–RN: 75–26–3
Group No.: 23–024
Molar Mass: 122.99

TABLE 23.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	298.0–317.7	4S	nosp	not specified		C_{avg}	DSIO	*81VON
50KUS/CRO	190.1–209.6	7	1.70	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.24.2. Correlated heat capacities

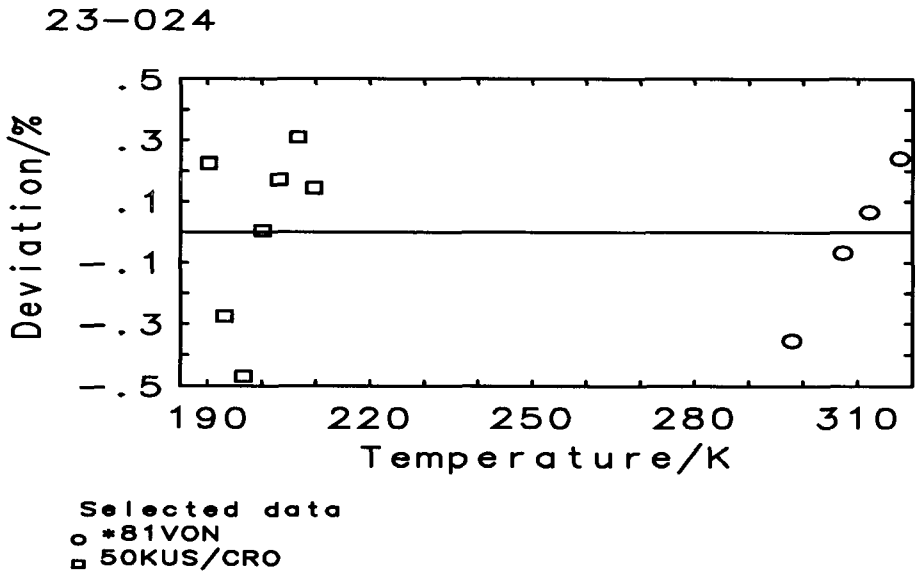
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	298.0–317.7	4	2.00#	0.110	3.51–2	0.22	–4.75–3	0
50KUS/CRO	190.1–209.6	7	1.70	0.156	4.01–2	0.27	2.24–3	2

TABLE 23.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.156	4.24–2	0.28	–3.04–4	2
Temp. range K		A_1	A_2				Level of uncertainty
190.1–317.7		1.34755+1	8.34816–1				V

TABLE 23.24.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.02	1.02	1.03	1.04	1.04	1.05	1.05
C_p (J K^{-1}mol^{-1})	125	126	127	127	128	129	129
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.06	1.06	1.07	1.07	1.07	1.08	1.08
C_p (J K^{-1}mol^{-1})	130	131	131	131	132	133	133
Temp. (K)	310	320					
c_p (J K^{-1}g^{-1})	1.09	1.09					
C_p (J K^{-1}mol^{-1})	134	134					



Name: 1–Bromobutane
Formula: C_4H_9Br

CAS–RN: 109–65–9
Group No.: 23–025
Molar Mass: 137.02

TABLE 23.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31DEE	176.9–292.3	27	nosp	not specified		C_p	BDAO	31DEE
48KUR	307.6–331.1	2	nosp	not specified		C_{avg}	DSIO	47KUR
49TSC/RIC3	298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1

TABLE 23.25.2. Correlated heat capacities

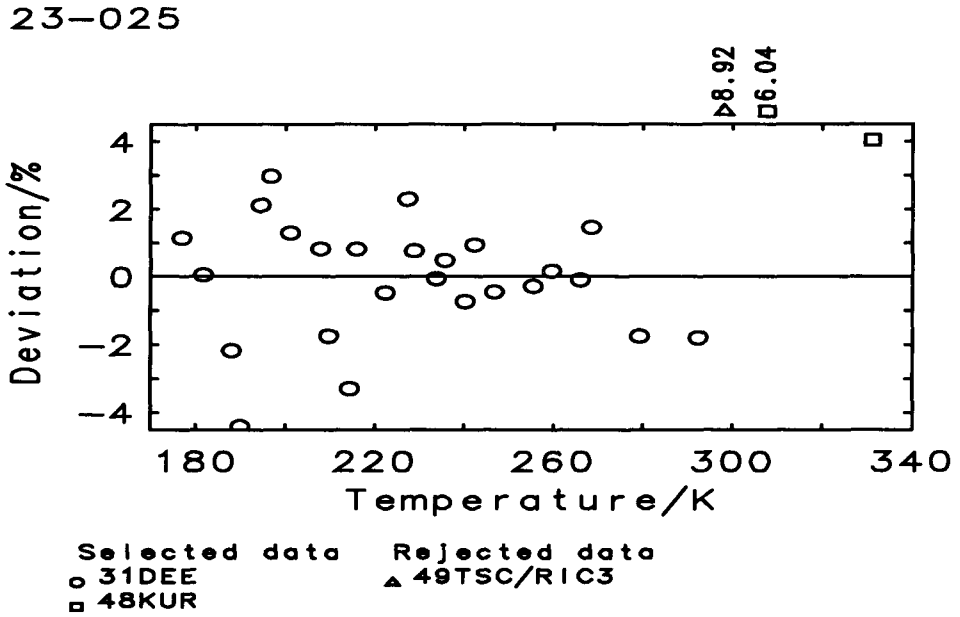
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31DEE	176.9–292.3	27	2.00#	0.830	2.80–1	1.66	–1.77–3	1
48KUR	307.6–331.1	2	5.00#	1.027	1.07	5.13	1.05	2
				Rejected data				
49TSC/RIC3	(1.85, 8.92, 1.85, 1)							

TABLE 23.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	30	29	0.893	4.12–1	2.21	7.11–2	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
176.9–331.1		2.67701+1	–9.71229	2.37252			V

TABLE 23.25.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.03	1.02	1.02	1.02	1.02	1.03	1.04
C_p (J K^{-1}mol^{-1})	141	140	140	140	140	141	142
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.05	1.07	1.08	1.09	1.10	1.13	1.15
C_p (J K^{-1}mol^{-1})	144	146	148	149	151	154	157
Temp. (K)	300	310	320	330			
c_p (J K^{-1}g^{-1})	1.15	1.18	1.21	1.25			
C_p (J K^{-1}mol^{-1})	158	162	166	171			



Name: 1–Bromo–2–methylpropane
Formula: C_4H_9Br

CAS–RN: 78–77–3
Group No.: 23–026
Molar Mass: 137.02

TABLE 23.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	306.1–319.1	2	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 23.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
306.1–319.1		7.64004	3.65968				VI

TABLE 23.26.4. Recommended values of heat capacities

Temp. (K)	310	320
c ($J K^{-1} g^{-1}$)	1.15	1.17
C ($J K^{-1} mol^{-1}$)	158	161

Name: 2–Bromo–2–methylpropane
Formula: C_4H_9Br

CAS–RN: 507–19–7
Group No.: 23–027
Molar Mass: 137.02

TABLE 23.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50KUS/CRO	259.6–265.1	3	2.00	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.062	2.24–2	0.12	1.84–5	1
Temp. range K		A_1	A_2				Level of uncertainty
259.6–265.1		1.58127+1	8.83802–1				V

TABLE 23.27.4. Recommended values of heat capacities

Temp. (K)	260	265
c_p (J K^{-1}g^{-1})	1.10	1.10
C_p (J K^{-1}mol^{-1})	151	151

Name: 1,3–Dibromo–2,2–bis(bromomethyl)propane
Formula: $C_5H_8Br_4$

CAS–RN: 3229–00–3
Group No.: 23–028
Molar Mass: 387.73

TABLE 23.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65CLE/WON	440.3–459.8	5	0.15	99.67	melpt	C_{sat}	BSAO	53WES/HAT

TABLE 23.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	5	0.296	1.67–2	0.04	–1.53–6	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
440.3–459.8		2.66935+2	–1.05536+2	1.21291+1			III

TABLE 23.28.4. Recommended values of heat capacities

Temp. (K)	440	450	460
c_{sat} (J K^{-1}g^{-1})	0.802	0.807	0.817
C_{sat} (J K^{-1}mol^{-1})	310.9	312.9	316.9

Name: 1–Bromo–3–methylbutane
Formula: $C_5H_{11}Br$

CAS–RN: 107–82–4
Group No.: 23–029
Molar Mass: 151.05

TABLE 23.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	306.9–330.3	2	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 23.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
306.9–330.3	7.74454	4.90486	VI

TABLE 23.29.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	1.26	1.29	1.32
C ($J\,K^{-1}mol^{-1}$)	191	195	199

Name: 1–Bromopentane
Formula: $C_5H_{11}Br$

CAS–RN: 110–53–2
Group No.: 23–030
Molar Mass: 151.05

TABLE 23.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31DEE	195.8–290.7	10	nosp	not specified		C_p	BDAO	31DEE
50KUS/CRO	190.1–206.6	6	1.50	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.30.2. Correlated heat capacities

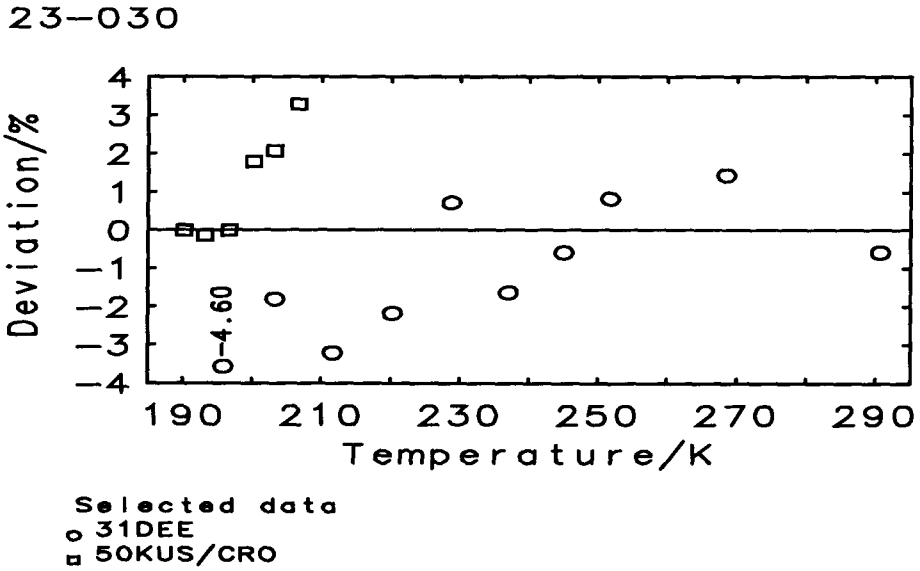
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
31DEE	195.8–290.7	10	2.00#	1.075	4.25–1	2.15	–2.28–1	–4
50KUS/CRO	190.1–206.6	6	1.50	1.165	3.66–1	1.75	2.44–1	2

TABLE 23.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	1.231	4.48–1	2.23	–5.12–2	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
190.1–290.7		3.46947+1	–1.22464+1	2.56531			V

TABLE 23.30.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1} g^{-1}$)	1.14	1.13	1.12	1.11	1.11	1.11	1.11
C_p ($J K^{-1} mol^{-1}$)	172	170	169	168	167	167	167
Temp. (K)	260	270	273.15	280	290	298.15	
c_p ($J K^{-1} g^{-1}$)	1.11	1.12	1.12	1.13	1.14	1.16	
C_p ($J K^{-1} mol^{-1}$)	168	169	169	171	173	174	



Name: 1,2–Dibromobenzene
Formula: $C_6H_4Br_2$

CAS–RN: 583–53–9
Group No.: 23–031
Molar Mass: 235.91

TABLE 23.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
18NAR	291.5–326.5	4S	nosp	not specified	C_{avg}	DSIO	18NAR

TABLE 23.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.035	3.97–2	0.18	6.77–5	0
Temp. range K		A_1	A_2				Level of uncertainty
291.5–326.5		1.41109+1	2.64264				VI

TABLE 23.31.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	0.77	0.78	0.78	0.79	0.80	0.80
C ($J K^{-1} mol^{-1}$)	181	183	183	185	188	190

Name: 1,3–Dibromobenzene
Formula: $C_6H_4Br_2$

CAS–RN: 108–36–1
Group No.: 23–032
Molar Mass: 235.91

TABLE 23.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
18NAR	290.9–326.4	4S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 23.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.105	1.16–1	0.52	6.10–4	0
Temp. range K		A_1	A_2				Level of uncertainty
290.9–326.4		1.43928+1	2.38844				VI

TABLE 23.32.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	0.75	0.76	0.76	0.77	0.78	0.79
C ($J K^{-1} mol^{-1}$)	177	179	179	181	183	185

Name: Bromobenzene
Formula: C_6H_5Br

CAS-RN: 108-86-1
Group No.: 23-033
Molar Mass: 157.01

TABLE 23.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		323.0–369.1	5S	nosp	not specified		C_{avg}	DSIO	*81VON
25WIL/DAN		293.1–353.1	4S	nosp	not specified		C_p	BSAO	24WIL/DAN
34KOL/UDO2	N	302.6	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
37STU		250.0–320.0	8S	nosp	not specified		C_p	BDHO	37STU
49TSC/RIC3		298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
75MAS/SCO		243.3–296.4	17	nosp	99.998	melpt	C_{sat}	BSAO	45SCO/MEY

34KOL/UDO2 same datum in 34KOL/UDO1

TABLE 23.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	323.0–369.1	5	2.00#	0.090	3.48–2	0.18	–1.82–2	–1
75MAS/SCO	243.3–296.4	17	0.20#	0.324	1.15–2	0.06	6.92–5	–1
				Rejected data				
25WIL/DAN	(4.98–1, 2.64, –4.72–1, –4)			34KOL/UDO2	(1.15, 6.60, –1.15, –1)			
37STU	(3.03–1, 1.65, 2.37–1, 6)			49TSC/RIC3	(4.99–1, 2.62, 4.99–1, 1)			

TABLE 23.33.3. Parameters of regression polynomial

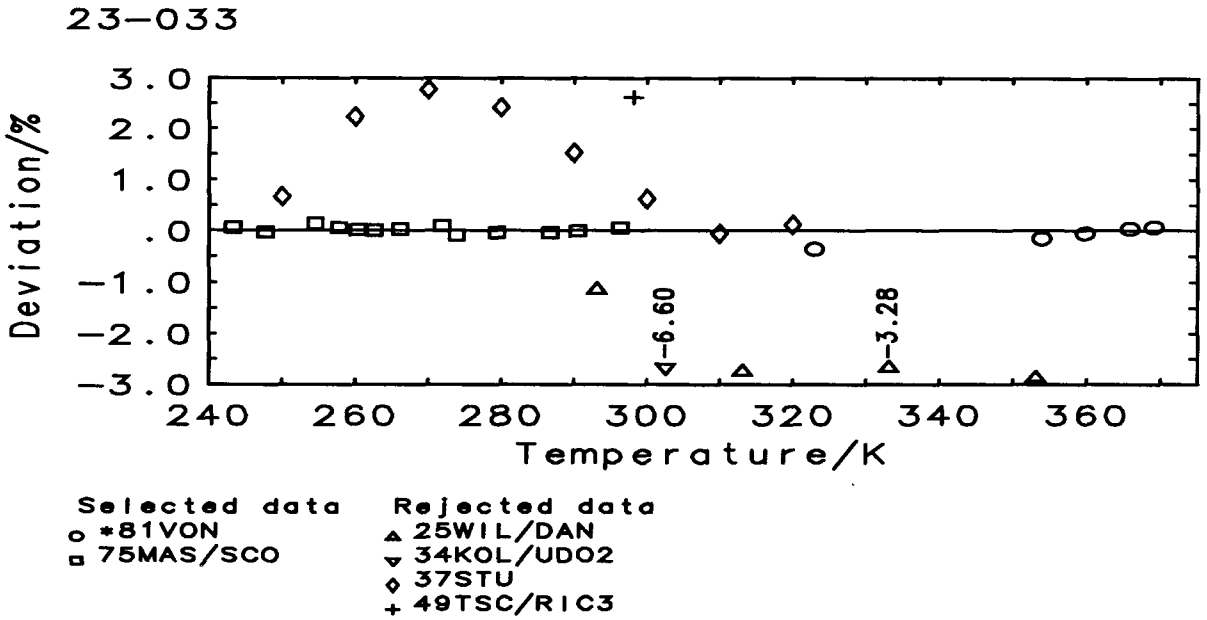
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	36	22	0.319	2.15–2	0.11	–4.09–3	–2
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
243.3–369.1	2.61761+1	–1.16331+1	4.40349	–4.56322–1			IV

TABLE 23.33.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c ($J K^{-1} g^{-1}$)	0.926	0.936	0.947	0.951	0.959	0.971	0.982
C ($J K^{-1} mol^{-1}$)	145.4	147.0	148.7	149.3	150.6	152.5	154.2
Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	0.984	0.998	1.011	1.024	1.038	1.051	1.063
C ($J K^{-1} mol^{-1}$)	154.5	156.6	158.7	160.8	162.9	164.9	166.9
Temp. (K)	370						
c ($J K^{-1} g^{-1}$)	1.075						
C ($J K^{-1} mol^{-1}$)	168.8						

TABLE 23.33.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	36	22	0.536	1.95–2	0.11	6.01–3	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
243.3–369.1	670.00	–4.09271	7.36012–1	1.22557+1	5.68953		IV



Name: 1–Bromohexane
Formula: $C_6H_{13}Br$

CAS–RN: 111–25–1
Group No.: 23–034
Molar Mass: 165.07

TABLE 23.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31DEE	214.0–289.8	12	nosp	not specified		C_p	BDAO	31DEE
49TSC/RIC3	298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1

TABLE 23.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
31DEE	214.0–289.8	12	2.00#	0.470	2.21–1	0.94	4.15–3	2

TABLE 23.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	12	0.515	2.42–1	1.03	4.15–3	2
Temp. range K		A_1	A_2				Level of uncertainty
214.0–289.8		1.95961+1	1.46585				V

TABLE 23.34.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1}g^{-1}$)	1.14	1.15	1.16	1.16	1.17	1.18	1.19
C_p ($J K^{-1}mol^{-1}$)	189	190	191	192	193	195	196
Temp. (K)	273.15	280	290	298.15			
c_p ($J K^{-1}g^{-1}$)	1.19	1.19	1.20	1.21			
C_p ($J K^{-1}mol^{-1}$)	196	197	198	199			

TABLE 23.34.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	12	0.543	2.55–1	1.09	4.15–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
214.0–289.8	629.00	–7.12945–1	1.59151–2	1.96982+1	7.98442		V

Name: 3–Bromohexane
Formula: $C_6H_{13}Br$

CAS–RN: 3377–87–5
Group No.: 23–035
Molar Mass: 165.07

TABLE 23.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88MEL/VER	213.1–523.2	10	2.50	not specified		C_{sat}	not specified	

TABLE 23.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.330	2.59–1	0.82	3.42–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
213.1–523.2		1.90435+1	4.36607	–1.80177	3.55138–1		V

TABLE 23.35.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.19	1.19	1.20	1.21	1.22	1.23	1.24
C_{sat} (J K^{-1}mol^{-1})	196	197	199	200	202	203	205
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.25	1.26	1.27	1.28	1.29	1.30	1.32
C_{sat} (J K^{-1}mol^{-1})	206	207	210	212	212	215	218
Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	1.34	1.36	1.38	1.41	1.44	1.47	1.50
C_{sat} (J K^{-1}mol^{-1})	221	225	228	233	237	242	247
Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	1.53	1.57	1.61	1.65	1.69	1.74	1.79
C_{sat} (J K^{-1}mol^{-1})	253	259	265	272	280	287	296
Temp. (K)	470	480	490	500	510	520	
c_{sat} (J K^{-1}g^{-1})	1.85	1.90	1.96	2.03	2.09	2.16	
C_{sat} (J K^{-1}mol^{-1})	305	314	324	334	346	357	

TABLE 23.35.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.552	3.88–1	1.38	6.16–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
213.1–523.2	608.00	–5.18058	1.98483	1.67436+1	3.38044		V

Name: 1–Bromoheptane
Formula: $C_7H_{15}Br$

CAS–RN: 629–04–9
Group No.: 23–036
Molar Mass: 179.10

TABLE 23.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
50CRO/SMY1	222.1–231.1	4	1.00	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.228	5.40–2	0.23	1.23–4	0
Temp. range K		A_1	A_2				Level of uncertainty
222.1–231.1		1.86821+1	2.18682				IV

TABLE 23.36.4. Recommended values of heat capacities

Temp. (K)	220	230
c_p ($J K^{-1} g^{-1}$)	1.091	1.101
C_p ($J K^{-1} mol^{-1}$)	195.3	197.2

Name: 1-Bromooctane
Formula: $C_8H_{17}Br$

CAS-RN: 111-83-1
Group No.: 23-037
Molar Mass: 193.13

TABLE 23.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50CRO/SMY1	222.1–234.1	3	1.00	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.093	2.91–2	0.09	3.50–5	-1

Temp. range K	A_1	Level of uncertainty
222.1–234.1	3.13671+1	IV

TABLE 23.37.4. Recommended values of heat capacities

Temp. (K)	220	230
c_p ($J K^{-1} g^{-1}$)	1.350	1.350
C_p ($J K^{-1} mol^{-1}$)	260.8	260.8

Name: 1-Bromononane
Formula: $C_9H_{19}Br$

CAS-RN: 693-58-3
Group No.: 23-038
Molar Mass: 207.15

TABLE 23.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50CRO/SMY1	248.6–257.1	4	1.00	not specified		C_p	BDHO	50KUS/CRO

TABLE 23.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	4	0.300	1.04–1	0.30	4.67–4	0

Temp. range K	A_1	Level of uncertainty
248.6–257.1	3.45579+1	IV

TABLE 23.38.4. Recommended values of heat capacities

Temp. (K)	250	260
c_p ($J K^{-1} g^{-1}$)	1.387	1.387
C_p ($J K^{-1} mol^{-1}$)	287.3	287.3

Name: 1–Bromodocosane
Formula: $C_{22}H_{45}Br$

CAS–RN: 6938–66–5
Group No.: 23–039
Molar Mass: 389.50

TABLE 23.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53HOF/DEC	318.1–333.1	3	4.00	90.	estim	C_p	BDHO	52HOF

TABLE 23.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.752	3.00	3.01	1.19–1	–1

Temp. range K	A_1	Level of uncertainty
318.1–333.1	9.85362+1	VI

TABLE 23.39.4. Recommended values of heat capacities

Temp. (K)	320	330
c_p ($J K^{-1} g^{-1}$)	2.10	2.10
C_p ($J K^{-1} mol^{-1}$)	819	819

Name: 1–Bromotriacontane
Formula: $C_{30}H_{61}Br$

CAS–RN: 4209–22–7
Group No.: 23–040
Molar Mass: 501.72

TABLE 23.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53HOF/DEC	343.1–353.1	2	4.00	90.	estim	C_p	BDHO	52HOF

TABLE 23.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
343.1–353.1		4.71744+1	2.52474+1				VI

TABLE 23.40.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p (J K^{-1}g^{-1})	2.20	2.25
C_p (J K^{-1}mol^{-1})	1110	1130

24. Iodine Derivatives

As iodine derivatives have not been studied with much frequency, there are only 9 such compounds in this family for which C_p data were reported at several temperatures.

For most compounds, the recommended data have been derived from old measurements (*81BER/OGI, *81VON, 18NAR) performed in German laboratories or they relate to studies at PTIL (48KUR) which are of limited and uncertain value, however, for many iodine compounds no other sources were available. The only extensive measurements with good accuracy (reported error of 0.5 %) were carried out for iodomethane at UCE (57HAR/MOE, 61LOW/MOE) and with somewhat lower accuracy for iodobenzene at JHUB (37STU, 61ROU) showing a reported error between 1 and 2 %.

Name: Diiodomethane
Formula: CH_2I_2

CAS-RN: 75-11-6
Group No.: 24-001
Molar Mass: 267.84

TABLE 24.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	307.1–363.0	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 24.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.062	5.20–2	0.31	9.35–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
307.1–363.0		1.02351+1	1.94967				VI

TABLE 24.1.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	0.51	0.51	0.52	0.52	0.53	0.54
C ($J K^{-1} mol^{-1}$)	135	137	139	140	142	143

Name: Iodomethane
Formula: CH_3I

CAS-RN: 74-88-4
Group No.: 24-002
Molar Mass: 141.94

TABLE 24.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	254.9–299.6	5	nosp	not specified		C_{avg}	DSIO	47KUR
57HAR/MOE	243.4–303.2	8	0.50	not specified		C_p	BSIO	57HAR/MOE
62LOW/MOE	253.2–308.2	7S	0.50	not specified		C_p	BSIO	57HAR/MOE

TABLE 24.2.2. Correlated heat capacities

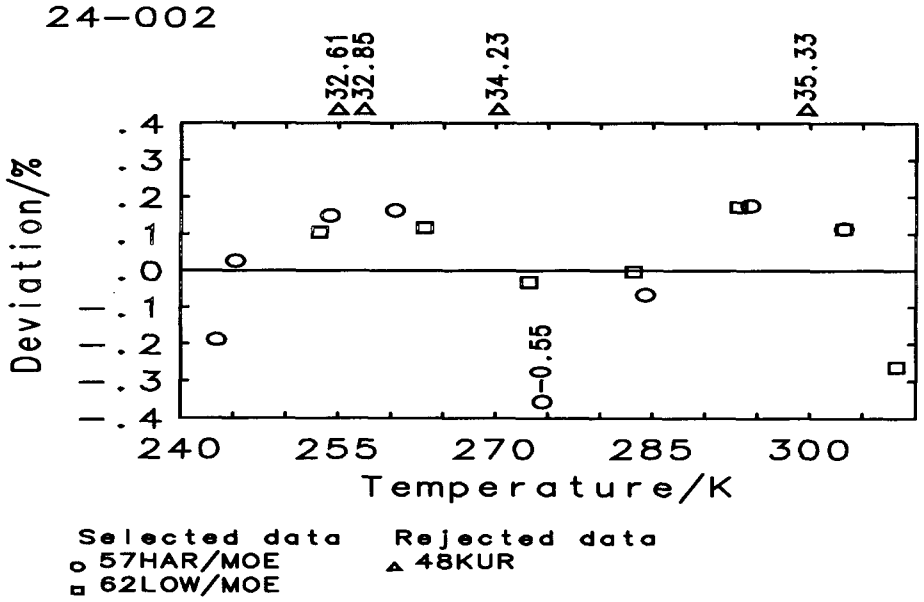
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57HAR/MOE	243.4–303.2	8	0.50	0.735	3.59–2	0.37	–8.09–3	–2
62LOW/MOE	253.2–308.2	7	0.50	0.446	2.19–2	0.22	9.65–3	3
				Rejected data				
48KUR	(4.98, 33.66, 4.97, 5)							

TABLE 24.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	15	0.457	2.24–2	0.23	6.74–5	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
243.4–308.2		–5.08573+1	7.25074+1	–2.87128+1	3.76706		IV

TABLE 24.2.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	0.577	0.575	0.573	0.571	0.571	0.571	0.575
C_p (J K^{-1}mol^{-1})	81.90	81.62	81.26	81.01	80.99	81.06	81.60
Temp. (K)	298.15	300	310				
c_p (J K^{-1}g^{-1})	0.581	0.583	0.598				
C_p (J K^{-1}mol^{-1})	82.53	82.82	84.89				



Name: Iodoethane
Formula: C_2H_5I

CAS-RN: 75-03-6
Group No.: 24-003
Molar Mass: 155.97

TABLE 24.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81BER/OGI	243.1–333.1	4S	nosp	not specified		C_{avg}	DSIO	*79BER
48KUR	263.4–316.6	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 24.3.2. Correlated heat capacities

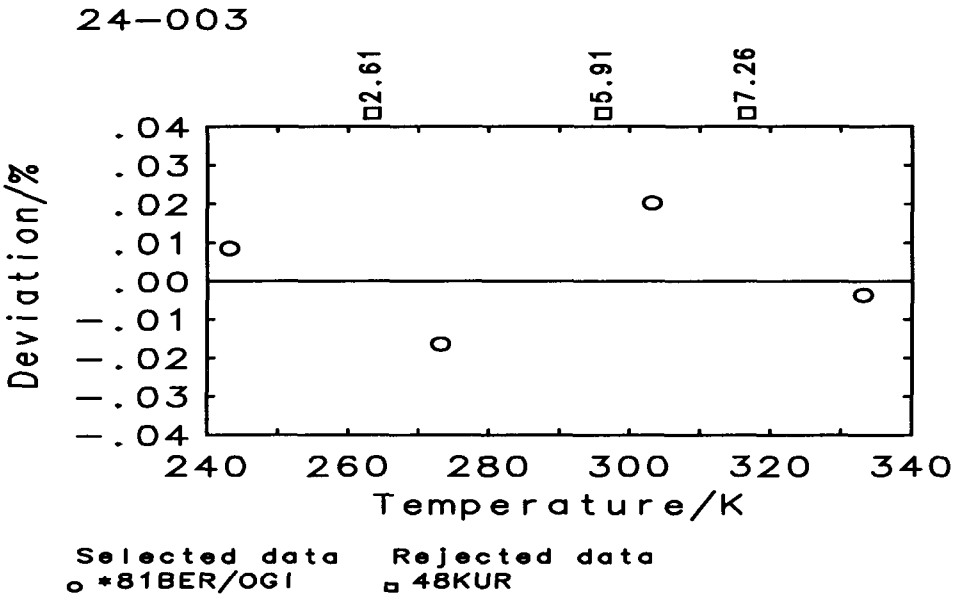
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81BER/OGI	243.1–333.1	4	5.00#	0.003	1.75–3	0.01	4.77–7	0
				Rejected data				
48KUR	(7.86–1, 5.61, 7.29–1, 3)							

TABLE 24.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	7	4	0.004	2.48–3	0.02	4.77–7	0
Temp. range K		A_1	A_2				Level of uncertainty
243.1–333.1		9.15537	1.29237				VI

TABLE 24.3.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1} g^{-1}$)	0.65	0.66	0.67	0.67	0.68	0.68	0.69
C ($J K^{-1} mol^{-1}$)	102	103	104	105	105	106	107
Temp. (K)	298.15	300	310	320	330		
c ($J K^{-1} g^{-1}$)	0.69	0.69	0.70	0.71	0.72		
C ($J K^{-1} mol^{-1}$)	108	108	109	111	112		



Name: 1–Iodopropane
Formula: C_3H_7I

CAS–RN: 107–08–4
Group No.: 24–004
Molar Mass: 169.99

TABLE 24.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	317.3–339.1	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 24.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.183	6.17–2	0.37	2.21–4	0
Temp. range K		A_1	A_2				Level of uncertainty
317.3–339.1		9.06545	2.40243				VI

TABLE 24.4.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J\,K^{-1}g^{-1}$)	0.82	0.83	0.84
C ($J\,K^{-1}mol^{-1}$)	139	141	143

Name: 1–Iodo–2–methylpropane
Formula: C_4H_9I

CAS–RN: 513–38–2
Group No.: 24–005
Molar Mass: 184.02

TABLE 24.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	315.0–344.5	3S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 24.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
315.0–344.5	2.05021+1	VI

TABLE 24.5.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J\,K^{-1}g^{-1}$)	0.93	0.93	0.93
C ($J\,K^{-1}mol^{-1}$)	170	170	170

Name: 1–Iodo–3–methylbutane
Formula: $C_5H_{11}I$

CAS–RN: 541–28–6
Group No.: 24–006
Molar Mass: 198.05

TABLE 24.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
48KUR	306.6–349.6	3	nosp	not specified		C_{avg}	DSIO	47KUR

TABLE 24.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.003	3.78–3	0.02	–1.91–6	1

Temp. range K	A_1	A_2	Level of uncertainty
306.6–349.6	8.53242	4.49787	VI

TABLE 24.6.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	0.94	0.96	0.98	1.00	1.02
C ($J\,K^{-1}mol^{-1}$)	187	191	194	198	202

Name: 1,2–Diiodobenzene
Formula: $C_6H_4I_2$

CAS–RN: 615–42–9
Group No.: 24–007
Molar Mass: 329.91

TABLE 24.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	297.0–325.2	3S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 24.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.009	1.07–2	0.05	3.82–6	1

Temp. range K	A_1	A_2	Level of uncertainty
297.0–325.2	1.80372+1	1.59961	VI

TABLE 24.7.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c ($J\,K^{-1}g^{-1}$)	0.58	0.58	0.58	0.59
C ($J\,K^{-1}mol^{-1}$)	190	191	193	194

Name: 1,3–Diiodobenzene
Formula: $C_6H_4I_2$

CAS–RN: 626–00–6
Group No.: 24–008
Molar Mass: 329.91

TABLE 24.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	321.9–340.0	2	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 24.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
321.9–340.0	1.39365+1	2.73652	VI

TABLE 24.8.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J\,K^{-1}g^{-1}$)	0.57	0.58	0.59
C ($J\,K^{-1}mol^{-1}$)	189	191	193

Name: Iodobenzene
Formula: C_6H_5I

CAS-RN: 591-50-4
Group No.: 24-009
Molar Mass: 204.01

TABLE 24.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
37STU	250.0–320.0	8S	nosp	not specified	C_p	BDHO	37STU
61ROU	301.3–316.2	7	nosp	not specified	C_p	BSAO	61ROU

TABLE 24.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37STU	250.0–320.0	8	2.00#	0.646	2.48–1	1.29	–1.48–1	–2
61ROU	301.3–316.2	7	1.00#	0.448	8.84–2	0.45	4.50–2	3

TABLE 24.9.3. Parameters of regression polynomial

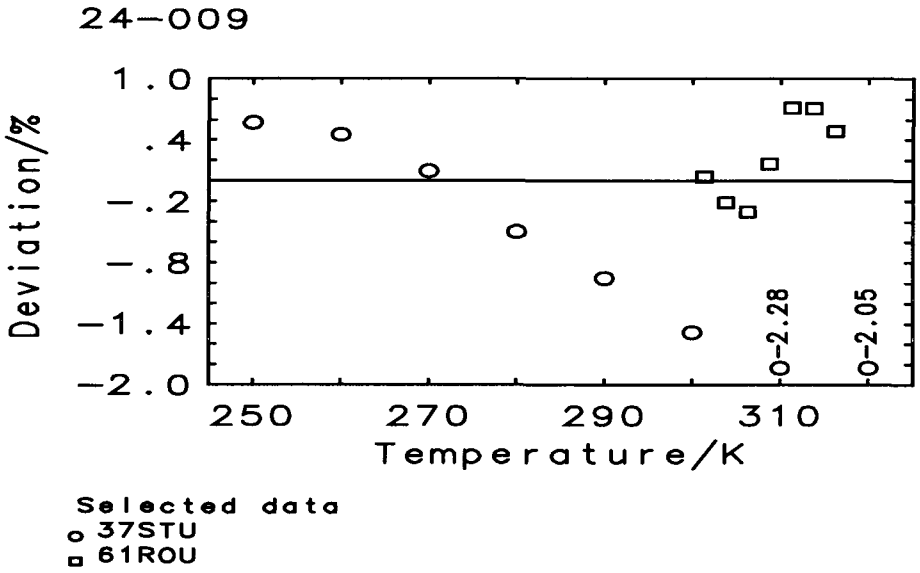
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.604	2.05–1	1.07	–5.81–2	1
Temp. range K		A_1	A_2				Level of uncertainty
250.0–320.0		1.42074+1	1.72619				V

TABLE 24.9.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	0.75	0.76	0.77	0.77	0.78	0.78	0.79
C_p (J K^{-1}mol^{-1})	154	155	157	157	158	160	161
Temp. (K)	300	310	320				
c_p (J K^{-1}g^{-1})	0.79	0.80	0.80				
C_p (J K^{-1}mol^{-1})	161	163	164				

TABLE 24.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.703	1.95–1	1.01	–1.54–2	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
250.0–320.0	721.20	6.14866–1	8.06828–3	1.47785+1	1.17144+1		V


24—009
1.0
.4
−.2
−.8
−1.4
−2.0
Deviation/%
250
270
290
310
Temperature/K
−2.28
−2.05
Selected data
37STU
61ROU

25. Mixed Halogen Derivatives

This mixed halogen family consists of 35 compounds containing at least two different halogen atoms of which two were measured at one temperature only.

Some of these mixed halogen compounds belong to the Freon refrigerants. A large number of measurements over a wide temperature and pressure range reflects the wide use and importance of Freons. The recommendations were made previously by Makita (77MAK) as parameters of polynomial expressing the temperature dependence for the recommended data of 14 Freons. The equations are based on a data compilation containing both experimental and estimated data.

The most extensive measurements (8 compounds, with a reported error 0.2 to 0.4 %) were performed at MSUM (71KOL/VOR, 72KOL/VOR, 74KOL/VOR, 74VOR/KOL, 78KOS/KOL, 81KOL/KOS, 82KOS/ZHO) over a wide temperature range and have been all included in the final correlation (with one exception 78KOS/KOL). Another laboratory reporting data on several mixed halogen derivatives is ICTP where 7 compounds were measured between 298 and 318 K with a reported error below 0.5 % (88SVO/VES, 88VES/ZAB).

Regarding substituted methanes, the interest was focused on $CBrF_3$ and $CClF_3$ (both refrigerants) which were investigated over a wide temperature and pressure range in an insufficiently identified Russian laboratory (84STO/CHA); the data were published as parameters of a correlating equation only. The compound, $CClF_3$, was also investigated at KITH (41RIE2). The reliability of both previous sources seems to be substantially lower than the claimed accuracy. Another compound investigated at KITH was CCl_2F_2 (39RIE3) and three other halogenated methane derivatives were measured up to above the normal boiling temperature at KCIW (40BEN/MCH), resulting in data with apparently low reliability. Other substituted methanes were measured at the following institutions: apparently high quality data for CCl_3F at CITP (41OSB/GAR); good quality data for $CHClF_2$ at OSU (57NEI/WHI) with a claimed error 0.5 % which seems to be realistic as well as data for $CHCl_2F$ along the saturation curve up to 0.65 MPa at ITN (74GRU/SHE). The latter data were reported as isobaric heat capacities and were converted to C_{sat} before the correlation procedure. From the last source, data were also obtained for 1,2-dibromo-1,1,2,2-tetrafluoroethane.

Beside the laboratories mentioned above, the halogenated ethanes were measured with good accuracy at PSC (55AST/WIL) for C_2ClF_5 and at UOTO (78KIS/SUG) for 1,1,2-trichloro-1,2,2-trifluoroethane over a narrow temperature range . The latter compound was measured and yielded results with lower accuracy but extended to high temperatures at KCIW (40BEN/MCH). Two additional ethane derivatives used as refrigerants were measured at KITH: unspecified isomer of $C_2Cl_2F_4$ (37PER1) and 1-chloro-1,1-difluoroethane (37PER1, 41RIE3). The data from 1941 have been discarded as better data were available in the same temperature range for the latter substance from LISI (64VAS2) with a reported error of 0.5 %. Two less common refrigerants R122 (1,1,2-trichloro-1,2-difluoroethane) and R132 (1,1-dichloro-1,2-difluoroethane) have been recently investigated over a wide temperature interval at CIUG (92LEB/KUL).

Regarding the derivatives of aromatic hydrocarbons, data are available for C_6BrF_5, C_6ClF_5 and 1,3,5-trichloro-2,4,6-trifluorobenzene measured at IICN (69PAU/GLU2, 75PAU2). In the case of the latter two compounds, more reliable data from NPLT (68AND/COU1, 73AND/MAR2) have been preferred as they differed substantially from the data obtained at IICN (by 1 and 3 % resp.) in the above reference.

Name: Bromotrichloromethane
Formula: $CBrCl_3$

CAS–RN: 75–62–7
Group No.: 25–001
Molar Mass: 198.27

TABLE 25.1.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59BEN/THO	298.00	0.7531	nosp	not specified		C_{avg}	BDHT	59BEN/THO

Name: Bromotrifluoromethane
Formula: $CBrF_3$

CAS–RN: 75–63–8
Group No.: 25–002
Molar Mass: 148.91

TABLE 25.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84STO/CHA	173.0–214.0	eqn	0.30	99.98	anal	C_p	BSAO	78SOL/SUK

TABLE 25.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.002	7.14–5	0.00	–5.09–7	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
173.0–213.6	7.36402	4.71839	–2.32916	5.28139–1	IV

TABLE 25.2.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210
c_p ($J\,K^{-1}g^{-1}$)	0.628	0.636	0.645	0.654	0.664
C_p ($J\,K^{-1}mol^{-1}$)	93.53	94.71	95.98	97.36	98.88

Name: Chlorotrifluoromethane
Formula: $CClF_3$

CAS–RN: 75–72–9
Group No.: 25–003
Molar Mass: 104.46

TABLE 25.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41RIE2	184.5–275.8	8	5.00	not specified		C_{sat}	BSIO	39RIE3
84STO/CHA	163.0–192.0	eqn	0.30	99.98	anal	C_p	BSAO	78SOL/SUK

TABLE 25.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
41RIE2	184.6–275.8	8	5.00	0.612	3.23–1	3.06	–2.08–1	–4
84STO/CHA	163.0–192.0	6	0.30	0.081	2.66–3	0.02	1.10–3	1

TABLE 25.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.551	2.89–1	2.74	–1.19–1	–3
C_{sat}	14	14	0.556	2.95–1	2.77	–1.11–1	–3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
163.0–275.8	–6.02362	2.62709+1	–1.46529+1	2.93097	V
163.0–275.8	5.20781–1	1.53838+1	–8.59481	1.80149	V

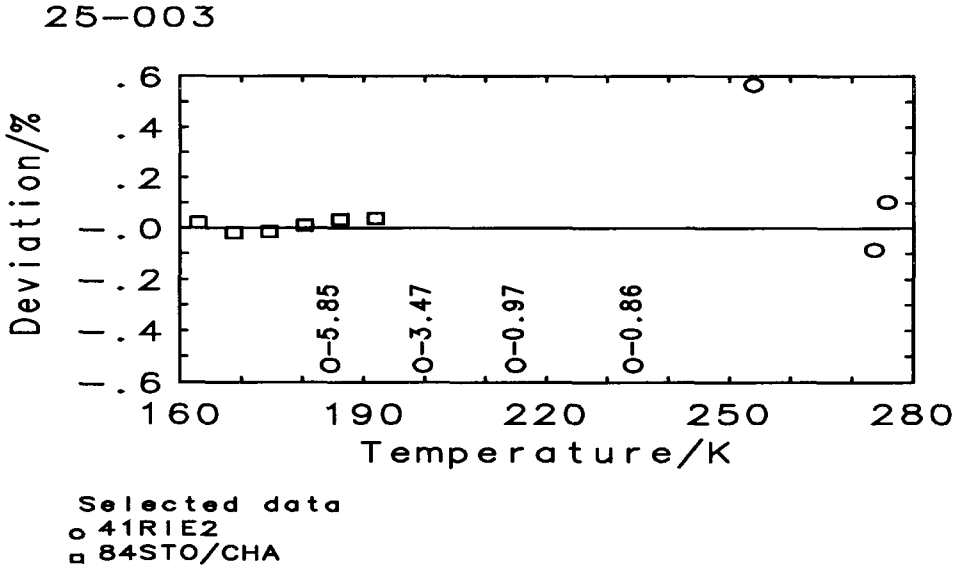
TABLE 25.3.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J K^{-1} g^{-1}$)	0.84	0.85	0.87	0.88	0.90	0.93	0.96
C_p ($J K^{-1} mol^{-1}$)	87.3	88.9	90.5	92.3	94.4	97.0	100
c_{sat} ($J K^{-1} g^{-1}$)	0.84	0.85	0.87	0.88	0.90	0.92	0.95
C_{sat} ($J K^{-1} mol^{-1}$)	87.4	88.8	90.4	92.1	94.1	96.5	99.3
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	1.00	1.05	1.10	1.17	1.26	1.28	1.35
C_p ($J K^{-1} mol^{-1}$)	104	109	115	123	131	134	141
c_{sat} ($J K^{-1} g^{-1}$)	0.98	1.02	1.07	1.12	1.18	1.20	1.25
C_{sat} ($J K^{-1} mol^{-1}$)	103	107	112	117	124	126	131

TABLE 25.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	10.330	3.45–1	3.19	1.63–1	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
163.0–275.8	302.00	–2.25339–1	2.90917–4	8.61948	1.06802+1	–3.29462+1	3.28366+1	V



Name: Dichlorodifluoromethane
Formula: CCl_2F_2

CAS–RN: 75–71–8
Group No.: 25–004
Molar Mass: 120.91

TABLE 25.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31BUF/FLE	N	230.1–290.1	2	4.00	not specified		C_{avg}	not specified	
39RIE3		194.4–293.5	12	1.00	not specified		C_{sat}	BSIO	39RIE3

31BUF/FLE the first datum from drop calorimetry; the second datum from isoperibol calorimetry

TABLE 25.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
39RIE3	194.4–293.5	12	1.00	0.456	5.95–2	0.46	5.54–4	2
				Rejected data				
31BUF/FLE	(9.39–1, 6.10, 6.53–1, 0)							

TABLE 25.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	12	0.526	6.86–2	0.53	5.54–4	2
C_{sat}	14	12	0.511	6.65–2	0.51	5.17–4	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
194.4–293.5	1.47834+1	–3.20041	1.01807	V
194.4–293.5	1.38976+1	–2.35789	8.18319–1	V

TABLE 25.4.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	0.85	0.86	0.86	0.87	0.88	0.89	0.90
C_p ($J\,K^{-1}mol^{-1}$)	103	104	104	105	106	108	109
c_{sat} ($J\,K^{-1}g^{-1}$)	0.85	0.86	0.86	0.87	0.88	0.89	0.90
C_{sat} ($J\,K^{-1}mol^{-1}$)	103	104	104	105	106	108	109
Temp. (K)	260	270	273.15	280	290	298.15	
c_p ($J\,K^{-1}g^{-1}$)	0.92	0.93	0.94	0.95	0.97	0.98	
C_p ($J\,K^{-1}mol^{-1}$)	111	113	113	115	117	119	
c_{sat} ($J\,K^{-1}g^{-1}$)	0.91	0.93	0.93	0.94	0.96	0.97	
C_{sat} ($J\,K^{-1}mol^{-1}$)	111	112	113	114	116	118	

TABLE 25.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	12	0.493	6.42–2	0.49	4.76–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
194.4–293.5	384.95	–7.73430–1	5.23607–1	1.06495+1	2.85612–1		V

Name: Trichlorofluoromethane
Formula: CCl_3F

CAS–RN: 75–69–4
Group No.: 25–005
Molar Mass: 137.37

TABLE 25.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
40BEN/MCH	261.4–347.5	4	nosp	not specified		C_{sat}	BSIO	40BEN/MCH
41OSB/GAR	170.6–287.8	13	0.10	99.95	melpt	C_{sat}	BSAO	41YOS/GAR

TABLE 25.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40BEN/MCH	261.5–347.5	4	1.50#	0.882	1.92–1	1.32	1.10–1	0
41OSB/GAR	170.6–287.8	13	0.10	0.260	3.63–3	0.03	–1.41–4	0

TABLE 25.5.3. Parameters of regression polynomial

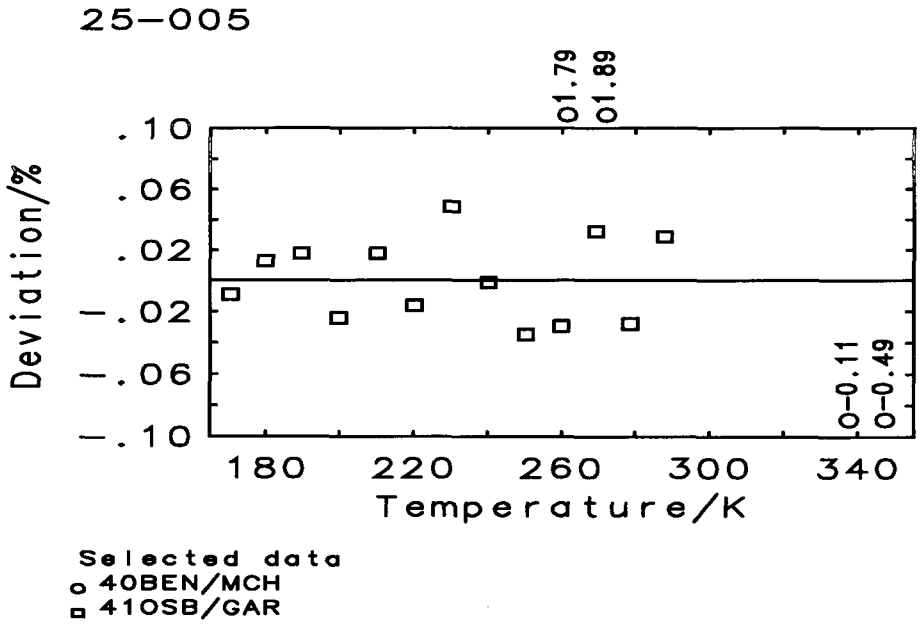
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.554	1.07–1	0.73	2.57–2	0
C_{sat}	17	17	0.548	1.07–1	0.74	2.56–2	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
170.6–347.5		1.09354+1	1.96990	–5.70283–1	1.09750–1		IV
170.6–347.5		1.12836+1	1.46261	–3.26291–1	7.10062–2		IV

TABLE 25.5.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	0.797	0.803	0.809	0.815	0.822	0.828	0.834
C_p (J K^{-1}mol^{-1})	109.5	110.4	111.2	112.0	112.9	113.7	114.6
c_{sat} (J K^{-1}g^{-1})	0.798	0.803	0.809	0.815	0.822	0.828	0.834
C_{sat} (J K^{-1}mol^{-1})	109.6	110.4	111.2	112.0	112.9	113.7	114.6
Temp. (K)	**240**	**250**	**260**	**270**	**273.15**	**280**	**290**
c_p (J K^{-1}g^{-1})	0.841	0.848	0.855	0.863	0.865	0.871	0.879
C_p (J K^{-1}mol^{-1})	115.5	116.5	117.5	118.5	118.9	119.6	120.8
c_{sat} (J K^{-1}g^{-1})	0.841	0.848	0.855	0.863	0.865	0.870	0.878
C_{sat} (J K^{-1}mol^{-1})	115.5	116.5	117.5	118.5	118.8	119.6	120.7
Temp. (K)	**298.15**	**300**	**310**	**320**	**330**	**340**	**350**
c_p (J K^{-1}g^{-1})	0.887	0.888	0.898	0.908	0.918	0.929	0.941
C_p (J K^{-1}mol^{-1})	121.8	122.0	123.3	124.7	126.1	127.7	129.3
c_{sat} (J K^{-1}g^{-1})	0.885	0.887	0.896	0.905	0.914	0.925	0.935
C_{sat} (J K^{-1}mol^{-1})	121.6	121.8	123.0	124.3	125.6	127.0	128.5

TABLE 25.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	4.809	9.84–2	0.70	2.01–2	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
170.6–347.5	471.20	–5.35921–1	1.44721–2	1.09985+1	4.96145		IV



Name: Chlorodifluoromethane
Formula: $CHClF_2$

CAS–RN: 75–45–6
Group No.: 25–006
Molar Mass: 86.47

TABLE 25.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
40BEN/MCH	255.8–328.3	4	nosp	not specified	C_{sat}	BSIO	40BEN/MCH
57NEI/WHI	121.8–226.1	12	0.50	99.98 melpt	C_p	BSIO	50JOH/CLA

TABLE 25.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40BEN/MCH	255.9–328.3	4	1.50#	0.537	1.11–1	0.81	4.72–2	2
57NEI/WHI	121.8–226.1	12	0.50	0.905	5.02–2	0.45	–1.19–3	0

TABLE 25.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.957	8.14–2	0.65	1.09–2	2
C_{sat}	16	16	0.909	7.54–2	0.64	1.43–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
121.8–328.3	8.15765	5.79995	–3.78720	8.07200–1	V
121.8–328.3	9.17639	3.96913	–2.71469	6.01885–1	V

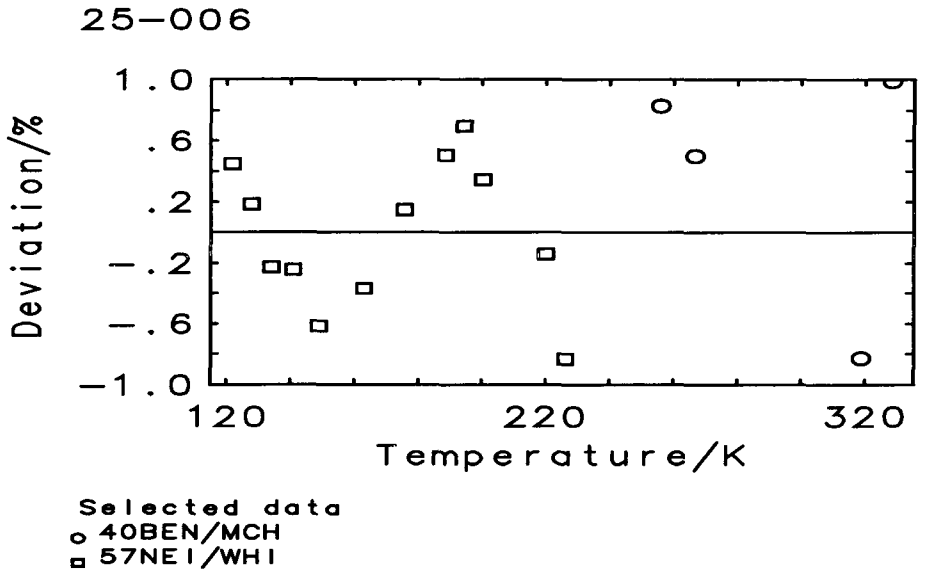
TABLE 25.6.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_p ($J\,K^{-1}g^{-1}$)	1.06	1.06	1.06	1.06	1.06	1.06	1.06
C_p ($J\,K^{-1}mol^{-1}$)	91.9	92.0	92.0	92.0	91.9	91.8	91.7
c_{sat} ($J\,K^{-1}g^{-1}$)	1.06	1.06	1.06	1.06	1.06	1.06	1.06
C_{sat} ($J\,K^{-1}mol^{-1}$)	92.0	92.0	92.0	91.9	91.8	91.8	91.8
Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	1.06	1.06	1.07	1.08	1.09	1.10	1.12
C_p ($J\,K^{-1}mol^{-1}$)	91.8	92.0	92.4	93.0	93.8	95.0	96.4
c_{sat} ($J\,K^{-1}g^{-1}$)	1.06	1.06	1.07	1.07	1.08	1.09	1.11
C_{sat} ($J\,K^{-1}mol^{-1}$)	91.8	92.0	92.4	92.9	93.7	94.7	95.9
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	1.14	1.16	1.17	1.19	1.23	1.27	1.28
C_p ($J\,K^{-1}mol^{-1}$)	98.3	101	101	103	107	110	110
c_{sat} ($J\,K^{-1}g^{-1}$)	1.13	1.15	1.16	1.17	1.21	1.23	1.24
C_{sat} ($J\,K^{-1}mol^{-1}$)	97.5	99.4	100	102	104	107	107
Temp. (K)	310	320	330				
c_p ($J\,K^{-1}g^{-1}$)	1.33	1.38	1.45				
C_p ($J\,K^{-1}mol^{-1}$)	115	120	125				
c_{sat} ($J\,K^{-1}g^{-1}$)	1.28	1.33	1.38				
C_{sat} ($J\,K^{-1}mol^{-1}$)	111	115	119				

TABLE 25.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	1.184	7.68–2	0.67	1.40–2	6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
121.8–328.3	369.30	–2.31206	7.97997–2	9.76315	6.63517	–2.42557+1	1.81513+1	V



Name: Dichlorofluoromethane
Formula: $CHCl_2F$

CAS–RN: 75–43–4
Group No.: 25–007
Molar Mass: 102.92

TABLE 25.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
40BEN/MCH		261.0–337.8	4	nosp	not specified		C_{sat}	BSIO	40BEN/MCH
74GRU/SHE	N	307.1–363.1	7S	1.00	99.77	chrom	C_p	BDHO	40TUR/BAR

74GRU/SHE C_p at saturation line (max. pressure 0.65 MPa)

TABLE 25.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
40BEN/MCH	261.0–337.9	4	1.50#	0.120	2.42–2	0.18	–6.40–3	0
74GRU/SHE	307.1–363.1	7	1.00	0.090	1.25–2	0.09	1.67–3	1

TABLE 25.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.119	2.07–2	0.15	–1.26–3	1
C_{sat}	11	11	0.093	1.70–2	0.13	–6.19–4	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
261.0–363.1	1.94294+1	–5.41461	1.08982	V
261.0–363.1	1.71561+1	–3.77772	7.94319–1	V

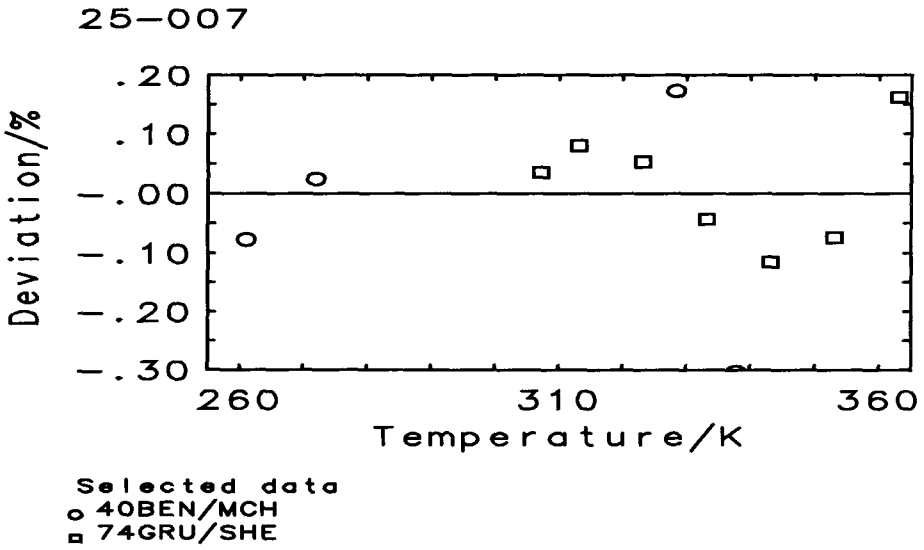
TABLE 25.7.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.03	1.03	1.03	1.04	1.04	1.05	1.05
C_p ($J K^{-1} mol^{-1}$)	106	106	106	107	107	108	108
c_{sat} ($J K^{-1} g^{-1}$)	1.03	1.03	1.03	1.03	1.04	1.05	1.05
C_{sat} ($J K^{-1} mol^{-1}$)	106	106	106	106	107	108	108
Temp. (K)	310	320	330	340	350	360	
c_p ($J K^{-1} g^{-1}$)	1.06	1.07	1.08	1.10	1.12	1.14	
C_p ($J K^{-1} mol^{-1}$)	109	110	112	113	115	117	
c_{sat} ($J K^{-1} g^{-1}$)	1.06	1.07	1.08	1.09	1.10	1.12	
C_{sat} ($J K^{-1} mol^{-1}$)	109	110	111	112	114	115	

TABLE 25.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.101	1.71–2	0.13	–1.74–3	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
261.0–363.1	451.60	–7.51806–2	5.13431–1	1.14156+1	2.75213–3	V



Name: 1,2–Dibromo–1,1,2,2–tetrafluoroethane
Formula: $C_2Br_2F_4$

CAS–RN: 124–73–2
Group No.: 25–008
Molar Mass: 259.82

TABLE 25.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74GRU/SHE	N	323.1–413.1	10S	1.00	99.995	chrom	C_p	BDHO	40TUR/BAR
82KOS/ZHO		165.7–297.0	25	nosp	99.46	melpt	C_{sat}	BSAO	79ZHO/KOS
88VES/ZAB		298.1–318.1	5	0.30	100.0	chrom	C_p	BSAO	79VES/ZAB

74GRU/SHE C_p at saturation line (max. pressure 1 MPa)

TABLE 25.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74GRU/SHE	323.1–413.1	10	1.00	1.520	3.41–1	1.52	1.35–1	2
82KOS/ZHO	165.7–297.0	25	0.40#	1.157	9.25–2	0.46	–3.05–2	–3
88VES/ZAB	298.1–318.1	5	0.30	1.424	8.96–2	0.43	6.63–2	3

TABLE 25.8.3. Parameters of regression polynomial

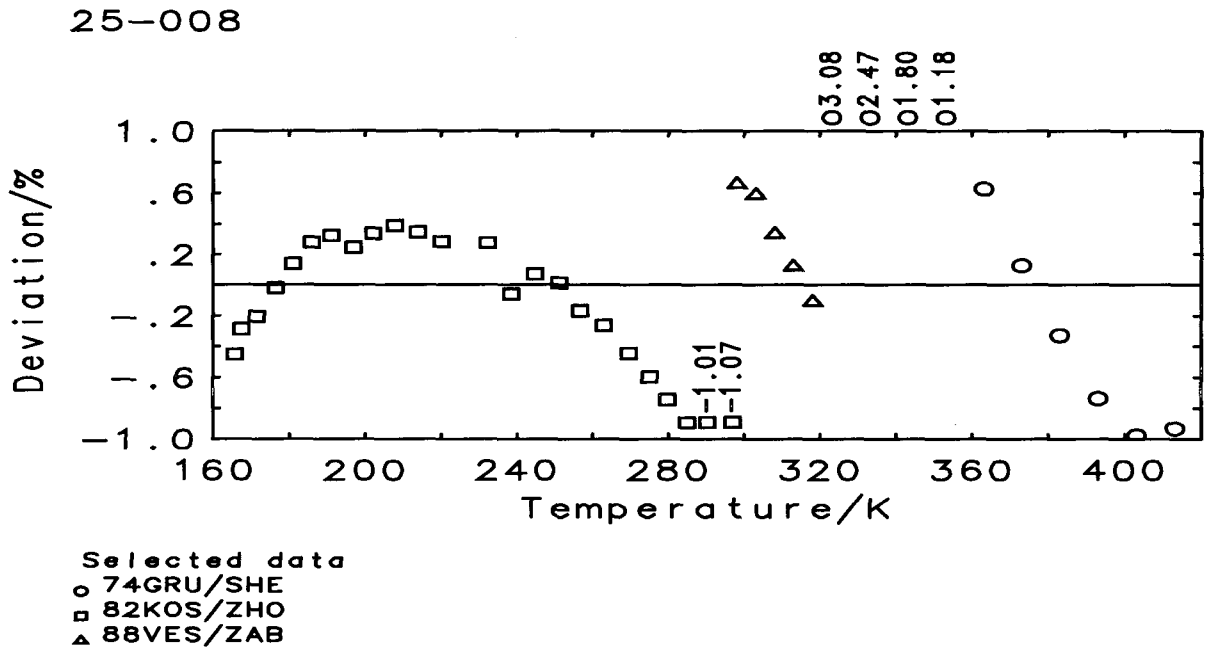
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	40	40	1.361	1.99–1	0.90	2.31–2	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
165.7–413.1		1.39894+1	3.97258	–1.18635	2.06692–1		IV

TABLE 25.8.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c ($J K^{-1}g^{-1}$)	0.587	0.592	0.598	0.603	0.608	0.614	0.620
C ($J K^{-1}mol^{-1}$)	152.4	153.8	155.3	156.7	158.1	159.5	161.0
Temp. (K)	240	250	260	270	273.15	280	290
c ($J K^{-1}g^{-1}$)	0.626	0.632	0.638	0.644	0.646	0.651	0.658
C ($J K^{-1}mol^{-1}$)	162.5	164.1	165.7	167.4	168.0	169.2	171.1
Temp. (K)	298.15	300	310	320	330	340	350
c ($J K^{-1}g^{-1}$)	0.665	0.666	0.674	0.682	0.691	0.701	0.711
C ($J K^{-1}mol^{-1}$)	172.7	173.0	175.1	177.3	179.7	182.1	184.8
Temp. (K)	360	370	380	390	400	410	
c ($J K^{-1}g^{-1}$)	0.722	0.733	0.745	0.758	0.772	0.787	
C ($J K^{-1}mol^{-1}$)	187.6	190.5	193.7	197.0	200.6	204.4	

TABLE 25.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	40	40	2.049	2.09–1	1.01	4.22–2	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
165.7–413.1	487.80	–1.81087	1.28482–1	1.49397+1	6.38073		V



Name: Chlorotrifluoroethene
Formula: C_2ClF_3

CAS–RN: 79–38–9
Group No.: 25–009
Molar Mass: 116.47

TABLE 25.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51OLI/GRI2	120.0–240.0	11S	0.20	99.84	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 25.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.247	6.75–3	0.05	3.03–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
120.0–240.0		1.81031+1	–7.41371	3.67702	–4.94745–1		II

TABLE 25.9.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_{sat} (J K^{-1}g^{-1})	0.974	0.970	0.969	0.970	0.973	0.978	0.984
C_{sat} (J K^{-1}mol^{-1})	113.5	113.0	112.9	113.0	113.3	113.9	114.6
Temp. (K)	190	200	210	220	230	240	
c_{sat} (J K^{-1}g^{-1})	0.992	1.001	1.011	1.022	1.034	1.046	
C_{sat} (J K^{-1}mol^{-1})	115.6	116.6	117.8	119.1	120.4	121.8	

TABLE 25.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	9	1.058	2.95–2	0.21	8.13–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
140.0–240.0	379.00	2.07355	1.84817	1.13435+1	5.81604–1		II

Name: Chloropentafluoroethane
Formula: C_2ClF_5

CAS–RN: 76–15–3
Group No.: 25–010
Molar Mass: 154.47

TABLE 25.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
55AST/WIL		175.0–230.0	12S	0.20	99.992	melpt	C_p	BSIO	36AST/MES
56PLA	N	303.1	1	nosp	not specified		C_{sat}	not specified	

56PLA original datum in Kinetic Chemicals Inc.Bulletin B–2, 1950

TABLE 25.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
55AST/WIL	175.0–230.0	12	0.20	0.530	1.76–2	0.11	–8.65–5	–1
56PLA	303.1	1	1.00#	0.169	3.81–2	0.17	3.81–2	1

TABLE 25.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	13	13	0.615	2.39–2	0.13	2.85–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
175.0–303.1		8.84825	9.09189	–4.95390	1.13497		III

TABLE 25.10.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c ($J K^{-1}g^{-1}$)	0.850	0.863	0.877	0.894	0.913	0.935	0.959
C ($J K^{-1}mol^{-1}$)	131.2	133.2	135.5	138.1	141.0	144.4	148.2
Temp. (K)	250	260	270	273.15	280	290	298.15
c ($J K^{-1}g^{-1}$)	0.988	1.020	1.056	1.069	1.097	1.143	1.184
C ($J K^{-1}mol^{-1}$)	152.6	157.5	163.1	165.1	169.5	176.5	182.9
Temp. (K)	300						
c ($J K^{-1}g^{-1}$)	1.194						
C ($J K^{-1}mol^{-1}$)	184.4						

Name: Dichlorotetrafluoroethane (unspecified isomer)
Formula: $C_2Cl_2F_4$

CAS-RN: 1320-37-2
Group No.: 25-011
Molar Mass: 170.92

TABLE 25.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
37PER1	N	183.1–293.3	26	nosp	not specified	C_{sat}	BSIO	37PER1

37PER1 mixture of two isomers, commercial product by Du Pont Co.; same data in 37PER2

TABLE 25.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	26	26	0.642	1.23–1	0.64	1.44–3	6
Temp. range K		A_1	A_2				Level of uncertainty
183.1–293.3		1.26750+1	2.69731				V

TABLE 25.11.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} ($J K^{-1}g^{-1}$)	0.85	0.87	0.88	0.89	0.91	0.92	0.93
C_{sat} ($J K^{-1}mol^{-1}$)	146	148	150	152	155	157	159
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J K^{-1}g^{-1}$)	0.94	0.96	0.97	0.97	0.98	1.00	1.01
C_{sat} ($J K^{-1}mol^{-1}$)	161	164	166	167	168	170	172

Name: 1,2–Dichloro–1,1,2,2–tetrafluoroethane
Formula: $C_2Cl_2F_4$

CAS–RN: 76–14–2
Group No.: 25–012
Molar Mass: 170.92

TABLE 25.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60MAR	N	237.1–275.9	2	nosp	not specified		C_{sat}	not specified	
81KOL/KOS		182.0–295.9	21	0.10	99.79	melpt	C_{sat}	BSAO	62KOL/SER

60MAR unpublished data: J.G.Aston, private communication (1955) and R.C.McHarness, private communication (1951)

TABLE 25.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
81KOL/KOS	182.0–295.9	21	0.10	1.388	2.51–2	0.14	7.14–5	–2
				Rejected data				
60MAR	(3.79–1, 1.95, 3.50–1, 2)							

TABLE 25.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	21	1.499	2.71–2	0.15	7.14–5	–2
C_{sat}	23	21	1.431	2.58–2	0.14	6.42–5	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
182.0–295.9	1.44940+1	8.20599–1	3.17576–1	III
182.0–295.9	1.41292+1	1.16680	2.36227–1	III

TABLE 25.12.4. Recommended values of heat capacities

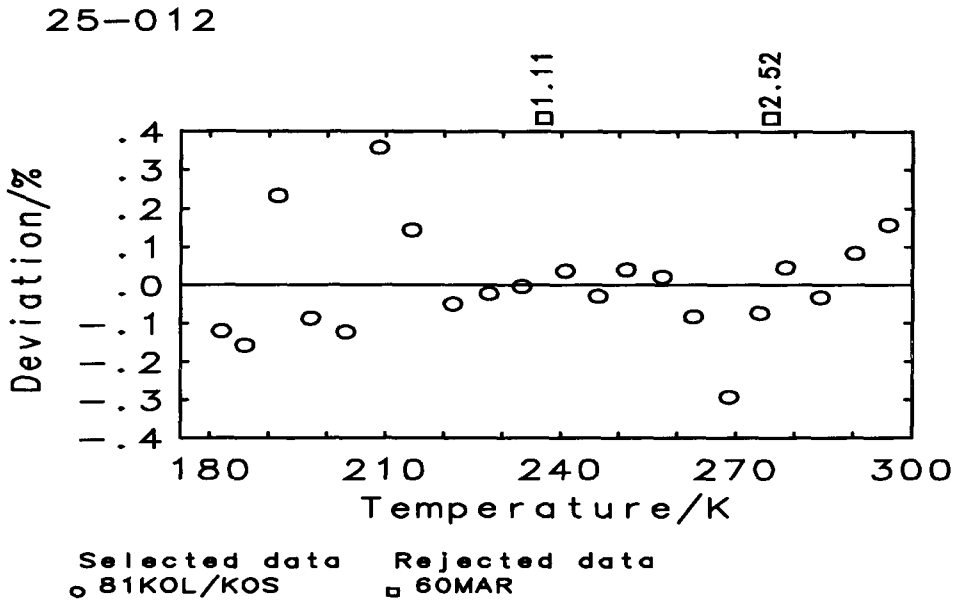
Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	0.827	0.837	0.847	0.857	0.868	0.879	0.890
C_p (J K^{-1}mol^{-1})	141.3	143.0	144.7	146.5	148.3	150.2	152.1
c_{sat} (J K^{-1}g^{-1})	0.827	0.837	0.847	0.857	0.868	0.879	0.890
C_{sat} (J K^{-1}mol^{-1})	141.3	143.0	144.7	146.5	148.3	150.2	152.1

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	0.901	0.913	0.925	0.929	0.938	0.951	0.961
C_p (J K^{-1}mol^{-1})	154.1	156.1	158.2	158.8	160.3	162.5	164.3
c_{sat} (J K^{-1}g^{-1})	0.901	0.913	0.924	0.928	0.936	0.949	0.959
C_{sat} (J K^{-1}mol^{-1})	154.0	156.0	158.0	158.6	160.0	162.1	163.9

Temp. (K)	300
c_p (J K^{-1}g^{-1})	0.964
C_p (J K^{-1}mol^{-1})	164.7
c_{sat} (J K^{-1}g^{-1})	0.961
C_{sat} (J K^{-1}mol^{-1})	164.3

TABLE 25.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	21	1.377	2.47–2	0.14	5.68–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
182.0–295.9	418.78	–1.53323	1.06437–1	1.35726+1	5.52154		III



Name: 1,1,1–Trichloro–2,2,2–trifluoroethane
Formula: $C_2Cl_3F_3$

CAS–RN: 354–58–5
Group No.: 25–013
Molar Mass: 187.38

TABLE 25.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88SVO/VES	298.1–318.1	5S	0.30	99.5	chrom	C_p	BSAO	79VES/ZAB

TABLE 25.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–318.1		1.31060+1	2.40543				III

TABLE 25.13.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	0.891	0.900	0.902	0.912	0.923
C_p ($J K^{-1}mol^{-1}$)	167.0	168.6	169.0	171.0	173.0

Name: 1,1,2–Trichloro–1,2,2–trifluoroethane
Formula: $C_2Cl_3F_3$

CAS–RN: 76–13–1
Group No.: 25–014
Molar Mass: 187.38

TABLE 25.14.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38RIE	N	242.9–333.9	19	0.50	not specified		C_{sat}	BSIO	39RIE3
40BEN/MCH		261.6–336.4	6	nosp	not specified		C_{sat}	BSIO	40BEN/MCH
54BUB	N	253.1–458.1	22S	3.30	not specified		C_p	BDAO	75RAS/GRI
81KOL/KOS		240.5–298.9	10	0.10	99.81	melpt	C_{sat}	BSAO	62KOL/SER
88VES/ZAB		298.1–318.1	5	0.30	100.0	chrom	C_p	BSAO	79VES/ZAB

38RIE same data in 39RIE1
54BUB C_p at saturation line extrapolated from high pressure measurements

TABLE 25.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
40BEN/MCH	261.6–336.5	6	1.50#	0.539	1.70–1	0.81	–2.05–2	2
54BUB	253.1–458.1	22	3.30	0.792	5.92–1	2.62	4.28–1	14
81KOL/KOS	240.5–298.9	10	0.10	1.019	2.08–2	0.10	1.47–3	0
88VES/ZAB	298.1–318.1	5	0.30	1.119	7.10–2	0.3	4–3.86–2	–1
				Rejected data				
38RIE	(5.66–1, 2.60, 5.18–1, 19)							

TABLE 25.14.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	43	0.920	4.57–1	2.02	2.12–1	15
C_{sat}	62	43	0.928	4.47–1	2.01	2.23–1	15

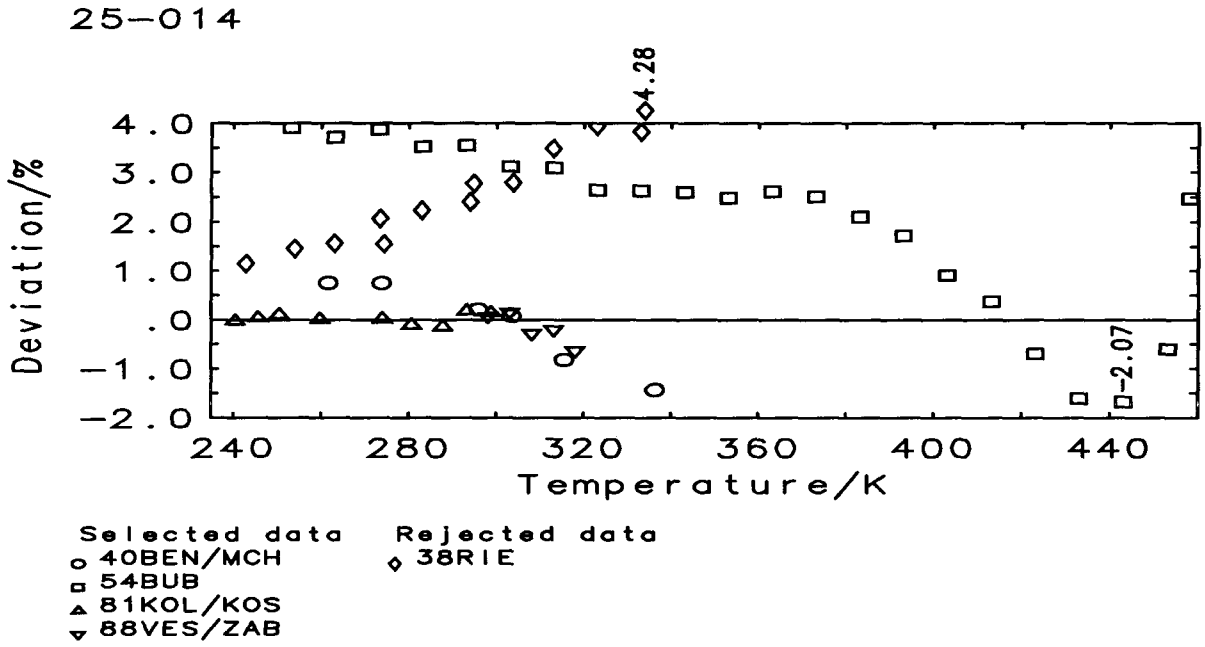
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
240.5–330.0	3.12424+1	–1.50403+1	5.63489	–5.92727–1	III
330.0–458.1	–9.79129+1	1.02374+2	–2.99451+1	3.00121	V
240.5–330.0	3.02747+1	–1.42054+1	5.42177	–5.79060–1	III
330.0–458.1	–7.62112+1	8.26000+1	–2.39132+1	2.38407	V

TABLE 25.14.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	0.861	0.870	0.879	0.889	0.893	0.901	0.912
C_p (J K^{-1}mol^{-1})	161.4	163.0	164.7	166.7	167.3	168.7	170.9
c_{sat} (J K^{-1}g^{-1})	0.861	0.870	0.879	0.890	0.893	0.901	0.912
C_{sat} (J K^{-1}mol^{-1})	161.4	163.0	164.7	166.7	167.3	168.7	170.9
Temp. (K)	298.15	300	310	320	330	340	350
c_p (J K^{-1}g^{-1})	0.922	0.924	0.937	0.949	0.962	0.97	0.99
C_p (J K^{-1}mol^{-1})	172.8	173.2	175.5	177.9	180.2	183	185
c_{sat} (J K^{-1}g^{-1})	0.922	0.924	0.936	0.948	0.960	0.97	0.98
C_{sat} (J K^{-1}mol^{-1})	172.7	173.1	175.4	177.6	179.8	182	184
Temp. (K)	360	370	380	390	400	410	420
c_p (J K^{-1}g^{-1})	1.00	1.02	1.04	1.06	1.09	1.12	1.16
C_p (J K^{-1}mol^{-1})	188	191	194	199	204	210	218
c_{sat} (J K^{-1}g^{-1})	1.00	1.01	1.03	1.05	1.07	1.10	1.13
C_{sat} (J K^{-1}mol^{-1})	187	190	193	196	201	206	212
Temp. (K)	430	440	450	460			
c_p (J K^{-1}g^{-1})	1.21	1.26	1.33	1.40			
C_p (J K^{-1}mol^{-1})	226	237	248	262			
c_{sat} (J K^{-1}g^{-1})	1.17	1.21	1.26	1.32			
C_{sat} (J K^{-1}mol^{-1})	219	227	237	248			

TABLE 25.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	43	7.769	3.32–1	1.54	–7.02–2	–11
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
240.5–458.1	487.30	–2.42293	3.01084–1	1.50316+1	4.87454		V



Name: 1,1,2,2–Tetrachloro–1,2–difluoroethane
Formula: $C_2Cl_4F_2$

CAS–RN: 76–12–0
Group No.: 25–015
Molar Mass: 203.83

TABLE 25.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
57YAR/KAY	305.0–353.0	eqn	1.10	not specified	C_p	BSIO	75PED/KAY
78KIS/SUG	299.0–310.3	5	0.30	99.93 melpt	C_p	BSAO	65SUG/SEK
78KOS/KOL	300.9–309.4	10	nosp	99.27 melpt	C_{sat}	BSAO	62KOL/SER

TABLE 25.15.2. Correlated heat capacities

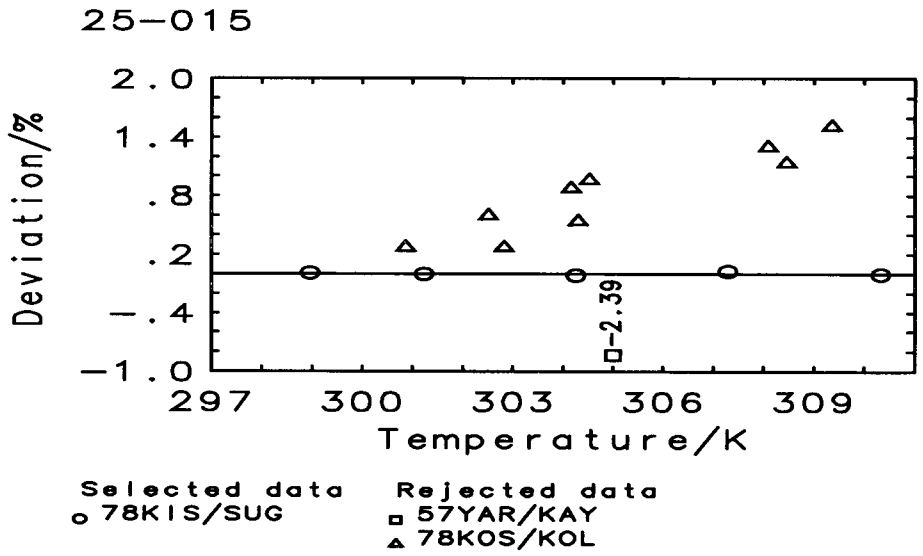
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
78KIS/SUG	299.0–310.3	5	0.30	0.048	3.09–3	0.01	0.00	0
				Rejected data				
57YAR/KAY	(5.03–1, 2.39, –5.03–1, –1)			78KOS/KOL	(1.93–1, 0.88, 1.68–1, 10)			

TABLE 25.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	5	0.062	3.98–3	0.02	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
299.0–310.3		1.60637+1	1.80535				III

TABLE 25.15.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p (J K^{-1}g^{-1})	0.876	0.884
C_p (J K^{-1}mol^{-1})	178.6	180.1



Name: 1–Bromo–2–chloro–1,1,2–trifluoroethane
Formula: $C_2HBrClF_3$

CAS–RN: 354–06–3
Group No.: 25–016
Molar Mass: 197.38

TABLE 25.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88VES/ZAB	298.1–318.1	5	0.30	99.0	chrom	C_p	BSAO	79VES/ZAB

TABLE 25.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.222	1.30–2	0.07	1.03–5	1

Temp. range K	A_1	A_2	Level of uncertainty
298.1–318.1	1.39079+1	1.80563	III

TABLE 25.16.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	0.806	0.813	0.814	0.822	0.829
C_p ($J K^{-1}mol^{-1}$)	159.2	160.4	160.7	162.2	163.7

Name: 2–Bromo–2–chloro–1,1,1–trifluoroethane
Formula: $C_2HBrClF_3$

CAS–RN: 151–67–7
Group No.: 25–017
Molar Mass: 197.38

TABLE 25.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88VES/ZAB	298.1–318.1	5	0.30	99.0	chrom	C_p	BSAO	79VES/ZAB

TABLE 25.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.255	1.46–2	0.08	1.30–5	2

Temp. range K	A_1	A_2	Level of uncertainty
298.1–318.1	1.29511+1	1.97094	III

TABLE 25.17.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	0.786	0.793	0.795	0.803	0.811
C_p ($J K^{-1}mol^{-1}$)	155.2	156.5	156.8	158.5	160.1

Name: 1,1,2–Trichloro–1,2–difluoroethane
Formula: $C_2HCl_3F_2$

CAS–RN: 354–15–4
Group No.: 25–018
Molar Mass: 169.38

TABLE 25.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
92LEB/KUL1	104.8–328.1	82	0.20	98.9	chrom	C_p	BSAO	76LEB/LIT

TABLE 25.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	82	82	2.630	1.21–2	0.53	1.22–4	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
104.8–328.1		2.68703	–7.19962–1	3.11068–1	–3.26272–2		III

TABLE 25.18.4. Recommended values of heat capacities

Temp. (K)	100	110	120	130	140	150	160
c_p (J K^{-1}g^{-1})	0.110	0.109	0.109	0.108	0.108	0.108	0.108
C_p (J K^{-1}mol^{-1})	18.67	18.53	18.41	18.33	18.29	18.27	18.27
Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	0.108	0.108	0.109	0.109	0.110	0.111	0.112
C_p (J K^{-1}mol^{-1})	18.31	18.36	18.44	18.54	18.66	18.80	18.95
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	0.113	0.114	0.115	0.116	0.117	0.117	0.119
C_p (J K^{-1}mol^{-1})	19.12	19.30	19.49	19.69	19.76	19.90	20.12
Temp. (K)	298.15	300	310	320	330		
c_p (J K^{-1}g^{-1})	0.120	0.120	0.121	0.123	0.124		
C_p (J K^{-1}mol^{-1})	20.29	20.34	20.56	20.78	21.00		

TABLE 25.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	82	82	4.535	2.09–2	0.91	3.54–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
104.8–328.1	525.10	1.32588	8.00097–1	1.38006	5.49299–1		IV

Name: 1,1–Dichloro–1,2–difluoroethane
Formula: $C_2H_2Cl_2F_2$

CAS–RN: 1842–05–3
Group No.: 25–019
Molar Mass: 134.94

TABLE 25.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
92LEB/KUL1	173.5–313.4	27	0.20	99.6	melpt	C_p	BSAO	76LEB/LIT

TABLE 25.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	26	1.453	6.15–3	0.29	3.15–5	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
173.5–307.6		2.09557	–1.31798–1	5.58456–2			III

TABLE 25.19.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	0.125	0.126	0.126	0.127	0.127	0.128	0.129
C_p (J K^{-1}mol^{-1})	16.90	16.96	17.02	17.09	17.17	17.26	17.36
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	0.129	0.130	0.131	0.132	0.133	0.133	0.135
C_p (J K^{-1}mol^{-1})	17.47	17.59	17.71	17.85	17.89	18.00	18.15
Temp. (K)	298.15	300	310				
c_p (J K^{-1}g^{-1})	0.135	0.136	0.137				
C_p (J K^{-1}mol^{-1})	18.28	18.32	18.49				

Name: 1–Chloro–1,1–difluoroethane
Formula: $C_2H_3ClF_2$

CAS–RN: 75–68–3
Group No.: 25–020
Molar Mass: 100.50

TABLE 25.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
37PER1	N	145.9–291.5	28	0.40	not specified		C_p	BSIO	37PER1
41RIE3	N	212.0–294.8	10	1.00	not specified		C_{sat}	BSIO	39RIE3
58CHE	N	245.1–370.1	15	nosp	not specified		C_{sat}	BSIO	58CHE
64VAS2		229.2–302.9	12	0.50	not specified		C_{sat}	BDAO	64VAS2

37PER1 same data in 37PER2
41RIE3 same data in 42RIE2
58CHE reproducibility given as 1–2 %

TABLE 25.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37PER1	145.9–291.5	28	1.50#	0.818	1.83–1	1.23	1.23–1	18
41RIE3	212.1–294.8	10	1.00	0.836	1.23–1	0.84	–7.26–2	–6
64VAS2	229.2–303.0	12	0.70#	0.546	5.69–2	0.38	–2.92–2	–4
				Rejected data				
58CHE	(8.16–1, 5.74, –8.00–1, –8)							

TABLE 25.20.3. Parameters of regression polynomial

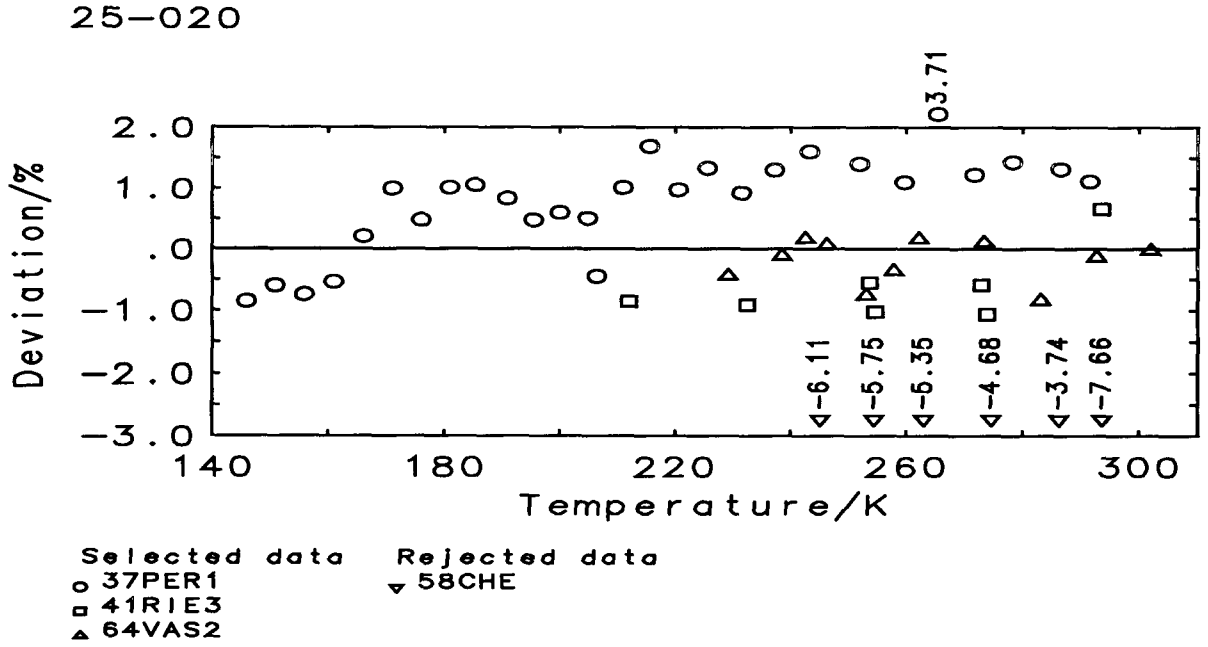
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	50	0.790	1.55–1	1.04	4.73–2	8
Temp. range K		A_1	A_2	A_3			Level of uncertainty
145.9–303.0		1.34379+1	–8.18832–1	5.28473–1			V

TABLE 25.20.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p ($J K^{-1} g^{-1}$)	1.11	1.12	1.12	1.13	1.14	1.15	1.16
C_p ($J K^{-1} mol^{-1}$)	111	112	113	114	115	116	117
Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J K^{-1} g^{-1}$)	1.17	1.19	1.20	1.22	1.23	1.25	1.25
C_p ($J K^{-1} mol^{-1}$)	118	119	121	122	124	125	126
Temp. (K)	280	290	298.15	300			
c_p ($J K^{-1} g^{-1}$)	1.26	1.28	1.30	1.30			
C_p ($J K^{-1} mol^{-1}$)	127	129	130	131			

TABLE 25.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	50	0.850	1.44–1	0.97	5.86–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
145.9–303.0	409.60	–1.39843	2.58966–1	1.16073+1	1.88789		V



Name: 1–Bromo–2–chloroethane
Formula: C_2H_4BrCl

CAS–RN: 107–04–0
Group No.: 25–021
Molar Mass: 143.41

TABLE 25.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
39RAI	N	262.5–321.5	11	2.00	99.8	melpt	C_p	BDHO	37STU

39RAI data from a graph only

TABLE 25.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.306	9.44–2	0.61	9.43–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
262.5–321.5		1.26695+1	9.70011–1				V

TABLE 25.21.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	0.88	0.89	0.89	0.89	0.90	0.90	0.90
C_p (J K^{-1}mol^{-1})	126	127	127	128	129	129	130
Temp. (K)	310	320					
c_p (J K^{-1}g^{-1})	0.91	0.91					
C_p (J K^{-1}mol^{-1})	130	131					

Name: 1–Chloro–1,1,3,3,3–pentafluoropropane
Formula: $C_3H_2ClF_5$

CAS–RN: 460–92–4
Group No.: 25–022
Molar Mass: 168.49

TABLE 25.22.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KOL/VOR		298.1	1	nosp	99.82	melpt	C_p	BSAO	62KOL/SER
74VOR/KOL	N	167.3–286.4	30	nosp	99.82	melpt	C_{sat}	BSAO	62KOL/SER

74VOR/KOL smoothed value at 298.15 K in 73KOL/VOR

TABLE 25.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KOL/VOR	298.1	1	0.40#	0.043	4.10–3	0.02	–4.10–3	–1
74VOR/KOL	167.3–286.4	30	0.40#	0.220	1.83–2	0.09	1.70–4	–4

TABLE 25.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	31	31	0.232	1.93–2	0.09	3.23–5	–5

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
167.3–298.1	2.23369+1	–4.94861	2.35063	–1.82728–1	III

TABLE 25.22.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c ($J\,K^{-1}g^{-1}$)	0.978	0.986	0.995	1.006	1.017	1.030	1.044
C ($J\,K^{-1}mol^{-1}$)	164.8	166.1	167.7	169.5	171.4	173.6	176.0
Temp. (K)	240	250	260	270	273.15	280	290
c ($J\,K^{-1}g^{-1}$)	1.060	1.076	1.093	1.111	1.117	1.130	1.150
C ($J\,K^{-1}mol^{-1}$)	178.5	181.3	184.2	187.2	188.2	190.4	193.7
Temp. (K)	298.15	300					
c ($J\,K^{-1}g^{-1}$)	1.166	1.170					
C ($J\,K^{-1}mol^{-1}$)	196.5	197.2					

Name: 1,1,1–Trichloro–3,3,3–trifluoropropane
Formula: $C_3H_2Cl_3F_3$

CAS–RN: 7125–84–0
Group No.: 25–023
Molar Mass: 201.40

TABLE 25.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KOL/VOR	246.3–296.8	6	0.20	99.59	melpt	C_{sat}	BSAO	62KOL/SER

TABLE 25.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	6	6	0.364	1.70–2	0.07	1.72–5	0
Temp. range K		A_1	A_2				Level of uncertainty
246.4–296.8		1.74468+1	2.21533				III

TABLE 25.23.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	0.949	0.958	0.967	0.970	0.976	0.985	0.993
C_{sat} (J K^{-1}mol^{-1})	191.1	193.0	194.8	195.4	196.6	198.5	200.0
Temp. (K)	300						
c_{sat} (J K^{-1}g^{-1})	0.995						
C_{sat} (J K^{-1}mol^{-1})	200.3						

Name: 3,3–Dichloro–1,1,1–trifluoropropane
Formula: $C_3H_3Cl_2F_3$

CAS–RN: 460–69–5
Group No.: 25–024
Molar Mass: 166.96

TABLE 25.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
72VOR/KOL	N	184.8–293.6	20	nosp	99.16	melpt	C_{sat}	BSAO	56POP/KOL

72VOR/KOL smoothed values in 72KOL/VOR

TABLE 25.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	20	20	0.341	3.05–2	0.14	7.07–5	–6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
184.8–293.6		2.20955+1	–1.92133	7.47765–1			III

TABLE 25.24.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.053	1.058	1.064	1.070	1.077	1.085	1.094
C_{sat} (J K^{-1}mol^{-1})	175.8	176.6	177.6	178.7	179.9	181.2	182.6
Temp. (K)	260	270	273.15	280	290		
c_{sat} (J K^{-1}g^{-1})	1.103	1.113	1.117	1.124	1.136		
C_{sat} (J K^{-1}mol^{-1})	184.2	185.9	186.5	187.7	189.7		

Name: 3–Chloro–1,1,1–trifluoropropane
Formula: $C_3H_4ClF_3$

CAS–RN: 460–35–5
Group No.: 25–025
Molar Mass: 132.51

TABLE 25.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74KOL/VOR	N	184.4–299.0	32	nosp	99.8	melpt	C_{sat}	BSAO	62KOL/SER

74KOL/VOR smoothed values in 72KOL/VOR

TABLE 25.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	32	32	0.628	3.71–2	0.19	1.27–4	–4

Temp. range K	A_1	A_2	A_3	Level of uncertainty
184.4–299.0	1.83387+1	–8.04779–1	5.19408–1	III

TABLE 25.25.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.165	1.172	1.180	1.188	1.197	1.207	1.217
C_{sat} (J K^{-1}mol^{-1})	154.4	155.4	156.4	157.5	158.7	159.9	161.3
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.228	1.240	1.252	1.256	1.265	1.278	1.290
C_{sat} (J K^{-1}mol^{-1})	162.7	164.3	165.9	166.4	167.6	169.4	170.9
Temp. (K)	300						
c_{sat} (J K^{-1}g^{-1})	1.292						
C_{sat} (J K^{-1}mol^{-1})	171.3						

Name: 1,4–Dibromo–2,3–dichloro–1,1,2,3,4,4–hexafluorobutane
Formula: $C_4Br_2Cl_2F_6$

CAS–RN: 375–42–8
Group No.: 25–026
Molar Mass: 392.75

TABLE 25.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88SVO/VES	298.1–318.1	5S	0.30	99.5	chrom	C_p	BSAO	79VES/ZAB

TABLE 25.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.067	7.28–3	0.02	2.29–6	0

Temp. range K	A_1	A_2	Level of uncertainty
298.1–318.1	2.59282+1	3.34333	III

TABLE 25.26.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	0.754	0.760	0.761	0.768	0.775
C_p ($J\,K^{-1}mol^{-1}$)	296.2	298.5	299.0	301.8	304.5

Name: Bromopentafluorobenzene
Formula: C_6BrF_5

CAS-RN: 344-04-7
Group No.: 25-027
Molar Mass: 246.96

TABLE 25.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75PAU2	245.9–281.5	6	nosp	99.9	melpt	C_{sat}	BSAO	69PAU/LAV2

TABLE 25.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	6	6	0.117	1.52–2	0.06	6.99–6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
245.9–281.5	3.32317+1	−7.85791	1.92818	IV

TABLE 25.27.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280
c_{sat} ($J\,K^{-1}g^{-1}$)	0.863	0.870	0.878	0.881	0.887
C_{sat} ($J\,K^{-1}mol^{-1}$)	213.2	214.8	216.8	217.5	219.1

Name: 1,6-Dibromo-2,3,5-trichloro-1,1,2,3,4,4,5,6,6-nonafluorohexane
Formula: $C_6Br_2Cl_3F_9$

CAS-RN: 85131-86-8
Group No.: 25-028
Molar Mass: 509.22

TABLE 25.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88SVO/VES	298.1–318.1	5S	0.30	99.5	chrom	C_p	BSAO	79VES/ZAB

TABLE 25.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.075	1.14–2	0.02	3.82–6	1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–318.1		4.03701+1	3.34342				III

TABLE 25.28.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	0.817	0.822	0.823	0.828	0.834
C_p ($J\,K^{-1}mol^{-1}$)	416.3	418.5	419.1	421.8	424.6

Name: Chloropentafluorobenzene
Formula: C_6ClF_5

CAS–RN: 344–07–0
Group No.: 25–029
Molar Mass: 202.51

TABLE 25.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
68AND/COU1	263.0–394.8	35	nosp	99.94	melpt	C_p	BSAO	63AND/COU1
69PAU/GLU2	263.8–302.7	14	nosp	98.89	melpt	C_p	BSAO	54STR/ICK

TABLE 25.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68AND/COU1	263.0–394.8	35	0.20#	0.227	1.23–2	0.05	1.13–5	5
				Rejected data				
69PAU/GLU2	(2.54–1, 0.96, 2.33–1, 12)							

TABLE 25.29.3. Parameters of regression polynomial

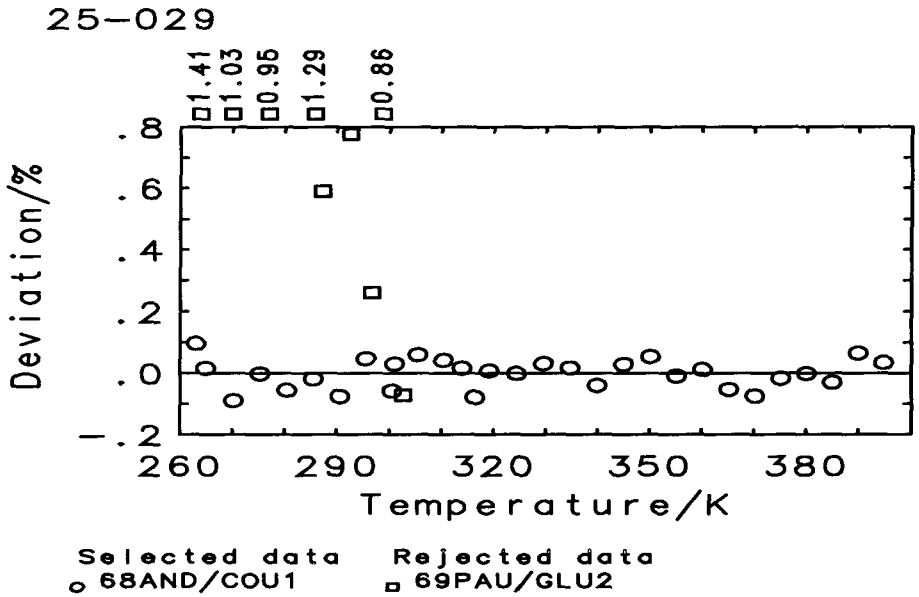
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	49	35	0.237	1.28–2	0.05	1.13–5	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
263.0–394.8		2.11722+1	1.17587	2.19901–1			II

TABLE 25.29.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.056	1.065	1.069	1.075	1.085	1.093	1.095
C_p ($J K^{-1} mol^{-1}$)	213.8	215.8	216.4	217.7	219.8	221.4	221.8
Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.106	1.116	1.127	1.138	1.149	1.160	1.171
C_p ($J K^{-1} mol^{-1}$)	223.9	226.0	228.2	230.4	232.7	234.9	237.2
Temp. (K)	380	390					
c_p ($J K^{-1} g^{-1}$)	1.183	1.195					
C_p ($J K^{-1} mol^{-1}$)	239.6	242.0					

TABLE 25.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	49	35	0.238	1.28–2	0.05	1.18–5	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
263.0–394.8	558.00	–1.82501	8.70882–2	1.99453+1	9.56122		II



Name: 1,3,5–Trichloro–2,4,6–trifluorobenzene
Formula: $C_6Cl_3F_3$

CAS–RN: 319–88–0
Group No.: 25–030
Molar Mass: 235.42

TABLE 25.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69PAU/GLU1	341.0–354.1	7	0.10	99.12	melpt	C_p	BSAO	54STR/ICK
73AND/MAR2	339.1–347.5	3	nosp	99.8	melpt	C_p	BSAO	63AND/COU1

TABLE 25.30.2. Correlated heat capacities

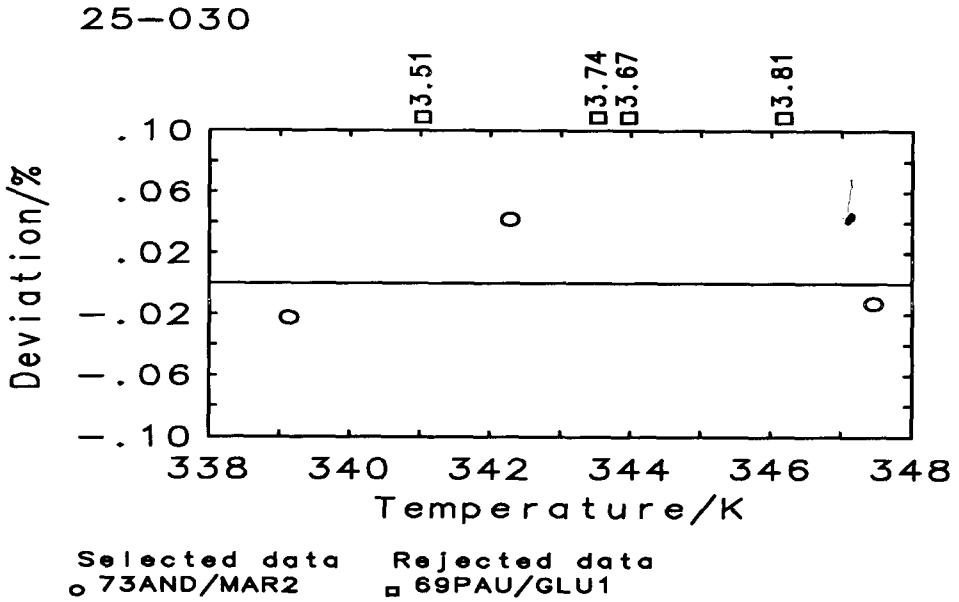
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73AND/MAR2	339.1–347.5	3	0.20#	0.141	8.07–3	0.03	5.09–6	–1
				Rejected data				
69PAU/GLU1	(1.09, 3.68, 1.09, 4)							

TABLE 25.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	3	0.245	1.40–2	0.05	5.09–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
339.1–347.5		1.87546+1	2.85573				II

TABLE 25.30.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.005	1.015
C_p ($J\,K^{-1}mol^{-1}$)	236.7	239.0



Name: 1–Bromo–2–chlorobenzene
Formula: C_6H_4BrCl

CAS–RN: 694–80–4
Group No.: 25–031
Molar Mass: 191.45

TABLE 25.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	306.0–326.3	4S	*nosp*	not specified		C_{avg}	DSIO	18NAR

TABLE 25.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.042	4.47–2	0.21	9.25–5	0
Temp. range K		A_1	A_2				Level of uncertainty
306.0–326.3		1.45410+1	2.25090				VI

TABLE 25.31.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	0.93	0.94	0.95
C ($J\,K^{-1}mol^{-1}$)	179	181	183

Name: 1–Bromo–3–chlorobenzene
Formula: C_6H_4BrCl

CAS–RN: 108–37–2
Group No.: 25–032
Molar Mass: 191.45

TABLE 25.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	254.3–326.5	4S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 25.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.071	7.63–2	0.35	2.83–4	0

Temp. range K	A_1	A_2	Level of uncertainty
254.3–326.5	1.44468+1	2.20624	VI

TABLE 25.32.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c ($J\,K^{-1}g^{-1}$)	0.88	0.89	0.89	0.90	0.91	0.91	0.91
C ($J\,K^{-1}mol^{-1}$)	168	170	170	171	173	175	175

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	0.92	0.93	0.94
C ($J\,K^{-1}mol^{-1}$)	177	179	181

Name: 1–Bromo–4–chlorobenzene
Formula: C_6H_4BrCl

CAS–RN: 106–39–8
Group No.: 25–033
Molar Mass: 191.45

TABLE 25.33.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	355.35	1.0000	nosp	not specified		C_{avg}	DSIO	18NAR

Name: 1–Bromo–2–iodobenzene
Formula: C_6H_4BrI

CAS–RN: 583–55–1
Group No.: 25–034
Molar Mass: 282.91

TABLE 25.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
18NAR	290.9–325.5	3S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 25.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.041	4.60–2	0.21	6.55–5	1
Temp. range K		A_1	A_2				Level of uncertainty
290.9–325.5		1.72090+1	1.69233				VI

TABLE 25.34.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	0.65	0.65	0.65	0.66	0.66	0.67
C ($J K^{-1} mol^{-1}$)	184	185	185	187	188	190

Name: 1–Bromo–3–iodobenzene
Formula: C_6H_4BrI

CAS–RN: 591–18–4
Group No.: 25–035
Molar Mass: 282.91

TABLE 25.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
18NAR	290.9–325.5	3S	nosp	not specified		C_{avg}	DSIO	18NAR

TABLE 25.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.023	2.53–2	0.11	1.97–5	1
Temp. range K		A_1	A_2				Level of uncertainty
290.9–325.5		1.63780+1	1.89294				VI

TABLE 25.35.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	0.64	0.65	0.65	0.65	0.66	0.66
C ($J K^{-1} mol^{-1}$)	182	183	183	185	187	188

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Heat Capacity of Liquids: Volume II Critical Review and Recommended Values

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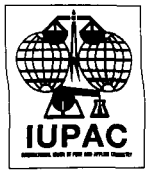

In association with the
International Union of Pure and Applied Chemistry
Commission on Thermodynamics

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31. Amines

The amine family contains 45 compounds of which 11 compounds were measured at one temperature only.

Many of the amines are of importance to chemical industry and considerable attention has been paid to their investigation by several research laboratories. BMB (now called NIPER) was the laboratory which carried out investigations on the largest number of amines (10 compounds) (72FIN/MES, 75MES/FIN, 81FIN/MES, 81MES/FIN, 86STE/CHI, 91STE/CHI); the reliability of data was high (reported error below 0.2 %) and the BMB data on amines have been in all cases included in the final correlation. Aminobiphenyl was measured recently at NIPER (91STE/CHI) up to the critical point using two different calorimeters; a low temperature adiabatic heat capacity and DSC calorimetry yielded results with reported errors of 0.1 and 1 %, respectively. Accurate measurements on three methyl amines were carried out at PSC (37AST/SIL, 39AST/EID2, 44AST/SAG). The results of other laboratories where several amines were investigated are, in general, of lower accuracy. Nevertheless, in many cases, these data had to be considered in the final correlation because of a lack of more reliable values. For certain compounds, data sets of limited reliability from different investigators have been included in the final correlation as it was not possible to decide which data should be preferred.

Some examples of striking discrepancies in the literature data for certain amines follow. Four aromatic amines (aniline, *N*-methylaniline, 1,3-diaminobenzene, 4,4'-diaminodiphenylmethane) were measured at LSCP (87LES/LIC) using a DSC instrument and gave data with a claimed error of 2 %. Only a third degree polynomial giving the C_p data as a function of temperature is presented by (87LES/LIC). However, for 1,3-diaminobenzene, the data from this source differ by 12 % from the values obtained at ANSM and GPI (84RAB/KAR) with a claimed error below 1.5 %. In the case of aniline, the published parameters of the correlation equation from the former source (87LES/LIC) even give negative values due to probable misprint in the parameters. The data by (88BOB/KAM) from an unidentified soviet laboratory for four di- through pentaamines have low reliability (claimed error of 6 %) as well as problems with the sample purity (3 % impurities reported). Nevertheless, in the case of 1,2-ethanediamine, the agreement was good with the reliable measurements from BMB (75MES/FIN) in the range where the data from both sources overlap. On the other hand, the data from CITP (50HOU/MAS2) for the same compound differ from the measurements of (75MES/FIN) by more than 3 % despite the low claimed error 0.4 % of the former data.

Di- and triethylamines were measured at IPCL (65KAU/BIT) with a flow calorimeter of their own construction with the claimed error of 1 %. While for diethylamine the agreement is excellent with the data obtained during excess heat capacity measurements at MGUM (85COS/PAT), it is difficult to select the best values for triethylamine. The data from IPCL are, in general, considerably higher numerically compared with the values obtained from excess heat capacity measurements. Therefore, in this case, all available data (except the old measurements *81VON) were included in the final correlation.

From an industrial standpoint, aniline is the most important chemical in the amine family. Two data sets were selected for establishing recommended values out of the 10 different measurements where data were obtained at several temperatures. Reliable data from DCM (62HAT/HIL) together with the high temperature data from CIPT (50HOU/MAS2) were used.

All other measurements with aromatic amines are from the older literature and were performed at universities in Germany (*81VON, *87SCH), Italy (*84BAT, 13CAM), and at YUNH (35SKA). On the basis of comparison with the other data, the probable error for the sources (*81VON, *87SCH) seems to be 2 to 3 %. Recent measurements at APIB (88GUS/MIR) differ from all other data for 2-methylaniline by more than 30 %. This was the main reason why we have discarded the data from the latter source. Also, the data were discarded for 3-methylaniline despite the fact that only two data points from different sources remained (34KOL/UDO1 and 90MEV/LIC). For the same reason, we have eliminated the heat capacities from RAB (78MAR/CIO1) derived from the enthalpy measurements; these results are not realistic and differ from other sources by about 100 %.

Name: Methanamine
Formula: CH_5N

CAS-RN: 74–89–5
Group No.: 31–001
Molar Mass: 31.06

TABLE 31.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
37AST/SIL	186.6–259.3	25	*nosp*	99.975 melpt	C_p	BSIO	36AST/MES

TABLE 31.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	1.055	5.13–2	0.42	3.96–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
186.6–259.3		1.10270+1	4.87486–1				III

TABLE 31.1.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	3.200	3.213	3.226	3.239	3.252	3.265	3.278
C_p ($J\,K^{-1}mol^{-1}$)	99.38	99.79	100.2	100.6	101.0	101.4	101.8
Temp. (K)	260						
c_p ($J\,K^{-1}g^{-1}$)	3.291						
C_p ($J\,K^{-1}mol^{-1}$)	102.2						

TABLE 31.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	1.005	4.88–2	0.40	3.45–4	–3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
186.6–259.3	430.70	9.73549	1.49904	7.94140	1.58068+1	III

Name: Ethanamine
Formula: C_2H_7N

CAS-RN: 75–04–7
Group No.: 31–002
Molar Mass: 45.08

TABLE 31.2.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
33POH/MEH	N	273.15	2.886	3.00	not specified	C_p	BSIO	33POH/MEH

33POH/MEH temperature not specified; estimated by the compilers

Name: *N*–Methylmethanamine
Formula: C_2H_7N

CAS–RN: 124–40–3
Group No.: 31–003
Molar Mass: 45.08

TABLE 31.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
39AST/EID2	184.8–280.5	20	0.10	99.989	melpt	C_p	BSAO	39AST/EID1

TABLE 31.3.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.559	9.01–3	0.06	7.87–6	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
184.8–230.0	–1.09101	1.05763+1	–1.89723–1	–5.10142–1	II
230.0–280.5	–6.17159+1	8.96522+1	–3.45705+1	4.47259	II

TABLE 31.3.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	2.733	2.807	2.869	2.919	2.955	2.979	2.994
C_p (J K^{-1}mol^{-1})	123.2	126.6	129.4	131.6	133.2	134.3	135.0

Temp. (K)	260	270	273.15	280
c_p (J K^{-1}g^{-1})	3.005	3.017	3.022	3.035
C_p (J K^{-1}mol^{-1})	135.5	136.0	136.2	136.9

TABLE 31.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	1.376	2.18–2	0.14	3.41–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
184.8–280.5	437.20	2.50684+2	2.33554+1	–6.52555+1	5.40026+2	–4.98427+2	5.01464+2	II

Name: 1,2–Ethanediamine
Formula: $C_2H_8N_2$

CAS–RN: 107–15–3
Group No.: 31–004
Molar Mass: 60.10

TABLE 31.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50HOU/MAS2	313.1–333.1	3S	0.40	99.8	estim	C_p	BSAO	50SAG/HOU
75MES/FIN	293.2–334.3	10	0.20	99.9	melpt	C_{sat}	BSAO	47HUF
88BOB/KAM	313.1–413.1	6	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 31.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75MES/FIN	293.3–334.3	10	0.20	0.097	4.03–3	0.02	8.83–5	–1
88BOB/KAM	313.1–413.1	6	6.00	0.176	2.19–1	1.06	–1.27–1	–2
				Rejected data				
50HOU/MAS2	(6.66–1, 3.07, 6.62–1, 3)							

TABLE 31.4.3. Parameters of cubic spline polynomials

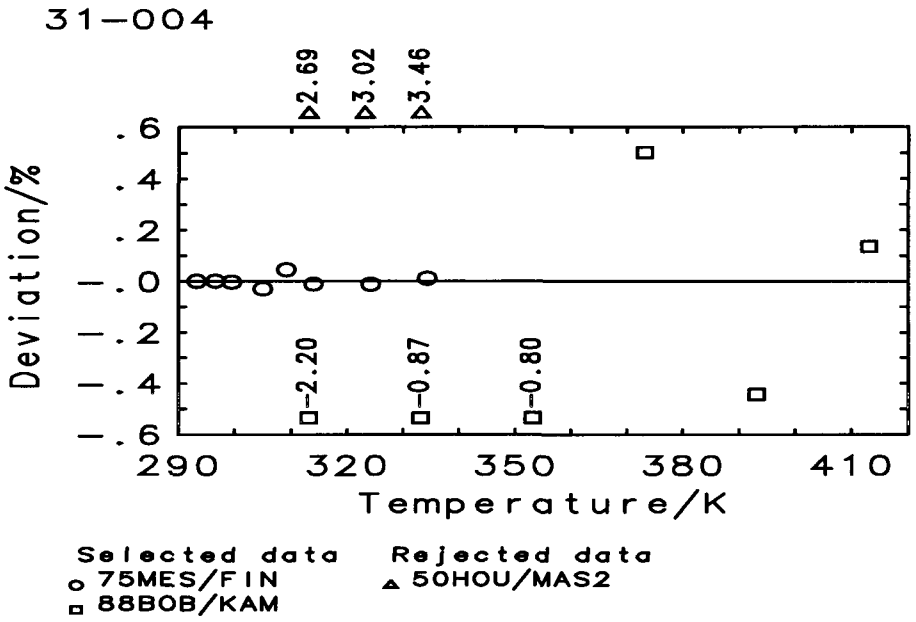
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	16	0.159	1.62–1	0.78	–4.74–2	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
293.2–350.0		3.49952+1	–1.41639+1	4.41414	–4.24354–1		II
350.0–413.1		–7.35765+2	6.46488+2	–1.84343+2	1.75526+1		VI

TABLE 31.4.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	2.863	2.872	2.874	2.887	2.901	2.916	2.931
C_{sat} (J K^{-1}mol^{-1})	172.1	172.6	172.7	173.5	174.3	175.2	176.2
Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	2.947	2.97	3.00	3.06	3.16	3.33	3.56
C_{sat} (J K^{-1}mol^{-1})	177.1	178	180	184	190	200	214

TABLE 31.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	16	1.223	2.92–1	1.32	–9.67–2	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
293.3–413.1	593.00	1.59683+2	4.38766+1	–2.89683+1	1.45285+2		V



Name: Cyclopropanamine
Formula: C_3H_7N

CAS–RN: 765–30–0
Group No.: 31–005
Molar Mass: 57.10

TABLE 31.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81FIN/MES	242.3–314.9	10	0.20	99.852	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 31.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.185	6.43–3	0.04	2.48–6	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
242.3–314.9		2.06413+1	–3.30496	7.77967–1			II

TABLE 31.5.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J $K^{-1}g^{-1}$)	2.503	2.511	2.520	2.532	2.537	2.546	2.563
C_{sat} (J $K^{-1}mol^{-1}$)	142.9	143.4	143.9	144.6	144.8	145.4	146.3
Temp. (K)	298.15	300	310				
c_{sat} (J $K^{-1}g^{-1}$)	2.578	2.582	2.603				
C_{sat} (J $K^{-1}mol^{-1}$)	147.2	147.4	148.6				

TABLE 31.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.222	7.71–3	0.04	4.58–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
242.3–314.9	512.00	6.23419	3.27899	1.35646+1	2.96319		II

Name: *N,N*–Dimethylmethanamine
Formula: C_3H_9N

CAS-RN: 75–50–3
Group No.: 31–006
Molar Mass: 59.11

TABLE 31.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
44AST/SAG	160.9–275.9	24	nosp	99.73	melpt	C_p	BSIO	36AST/MES

TABLE 31.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	24	0.493	2.18–2	0.15	5.40–5	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
160.9–275.9		1.64309+1	–3.52861	1.20720			II

TABLE 31.6.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J\,K^{-1}g^{-1}$)	1.952	1.958	1.968	1.981	1.998	2.018	2.041
C_p ($J\,K^{-1}mol^{-1}$)	115.4	115.7	116.3	117.1	118.1	119.3	120.7
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	2.068	2.098	2.132	2.169	2.209	2.222	2.253
C_p ($J\,K^{-1}mol^{-1}$)	122.2	124.0	126.0	128.2	130.6	131.4	133.2

TABLE 31.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	24	0.796	3.52–2	0.24	1.40–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
160.9–275.9	432.80	3.99251	3.40762	9.83020	1.16945		II

Name: 1–Propanamine
Formula: C_3H_9N

CAS–RN: 107–10–8
Group No.: 31–007
Molar Mass: 59.11

TABLE 31.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67SMI/GOO2	298.1	1	nosp	99.972	melpt	C_p	not specified	
71KON/WAD	298.1	1	nosp	99.8	estim	C_p	BSIO	70LKB/COM
71VAS/PET	187.8–302.4	52	nosp	not specified		C_p	BSAO	77KU/COM
72FIN/MES	190.0–334.6	19	0.20	99.972	melpt	C_{sat}	BSAO	47HUF

TABLE 31.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67SMI/GOO2	298.1	1	0.30#	0.142	8.33–3	0.04	–8.33–3	–1
72FIN/MES	190.0–334.6	19	0.20	0.067	2.57–3	0.01	1.96–4	2
				Rejected data				
71KON/WAD	(3.08–1, 1.60,–3.08–1, –1)			71VAS/PET	(3.75–1, 1.91, 3.13–1, 44)			

TABLE 31.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	73	20	0.081	3.49–3	0.02	–2.31–4	1
C_{sat}	73	20	0.077	3.39–3	0.02	–2.42–4	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
190.0–334.6	5.92272	1.40946+1	–5.20603	6.74771–1	II
190.0–334.6	6.25752	1.36481+1	–5.00907	6.46022–1	II

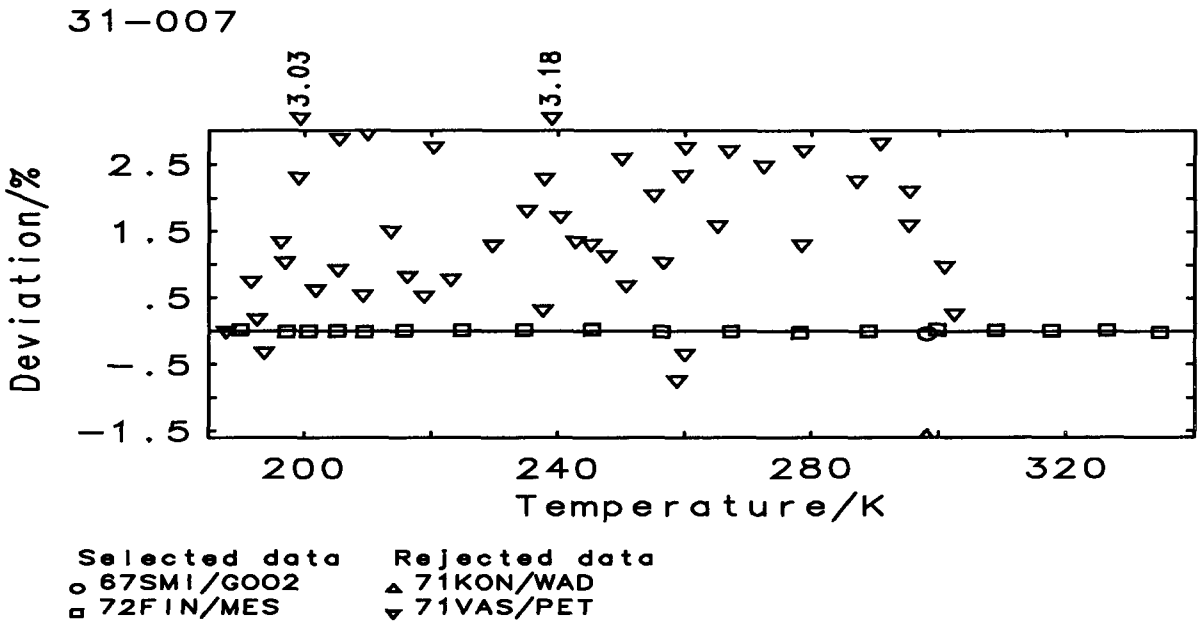
TABLE 31.7.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	2.607	2.628	2.646	2.661	2.674	2.685	2.696
C_p (J K^{-1}mol^{-1})	154.1	155.4	156.4	157.3	158.1	158.7	159.3
c_{sat} (J K^{-1}g^{-1})	2.607	2.628	2.646	2.661	2.674	2.685	2.696
C_{sat} (J K^{-1}mol^{-1})	154.1	155.4	156.4	157.3	158.1	158.7	159.4
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.706	2.716	2.719	2.727	2.739	2.750	2.753
C_p (J K^{-1}mol^{-1})	159.9	160.5	160.7	161.2	161.9	162.6	162.7
c_{sat} (J K^{-1}g^{-1})	2.706	2.716	2.719	2.726	2.738	2.749	2.752
C_{sat} (J K^{-1}mol^{-1})	159.9	160.5	160.7	161.2	161.9	162.5	162.7
Temp. (K)	310	320	330				
c_p (J K^{-1}g^{-1})	2.769	2.789	2.812				
C_p (J K^{-1}mol^{-1})	163.7	164.8	166.2				
c_{sat} (J K^{-1}g^{-1})	2.767	2.786	2.808				
C_{sat} (J K^{-1}mol^{-1})	163.6	164.7	166.0				

TABLE 31.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	73	20	1.180	4.57–2	0.24	–2.87–3	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
190.0–334.6	497.00	–1.03396	1.64111–1	1.72535+1	1.62857	III



Name: 2–Propanamine
Formula: C_3H_9N

CAS–RN: 75–31–0
Group No.: 31–008
Molar Mass: 59.11

TABLE 31.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
50HOU/MAS2	313.1–343.1	4	0.40	99.8	estim	C_p	BSAO	50SAG/HOU
67SMI/GOO2	298.1	1	nosp	99.992	melpt	C_p	not specified	
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM
72FIN/MES	181.5–318.2	18	0.20	99.993	melpt	C_{sat}	BSAO	47HUF

TABLE 31.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50HOU/MAS2	313.1–343.1	4	0.40	1.456	1.15–1	0.58	–7.05–2	–2
71KON/WAD	298.1	1	0.50#	0.194	1.91–2	0.10	1.91–2	1
72FIN/MES	181.5–318.2	18	0.20	0.287	1.13–2	0.06	3.83–3	3
				Rejected data				
67SMI/GOO2	(1.94–1, 0.98, 1.94–1, 1)							

TABLE 31.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	23	0.725	5.42–2	0.27	–8.43–3	2
C_{sat}	24	23	0.723	5.38–2	0.27	–8.50–3	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
181.5–343.1	–3.92944	2.37755+1	–8.42076	1.04149	II
181.5–343.1	–3.43523	2.30982+1	–8.11393	9.95545–1	II

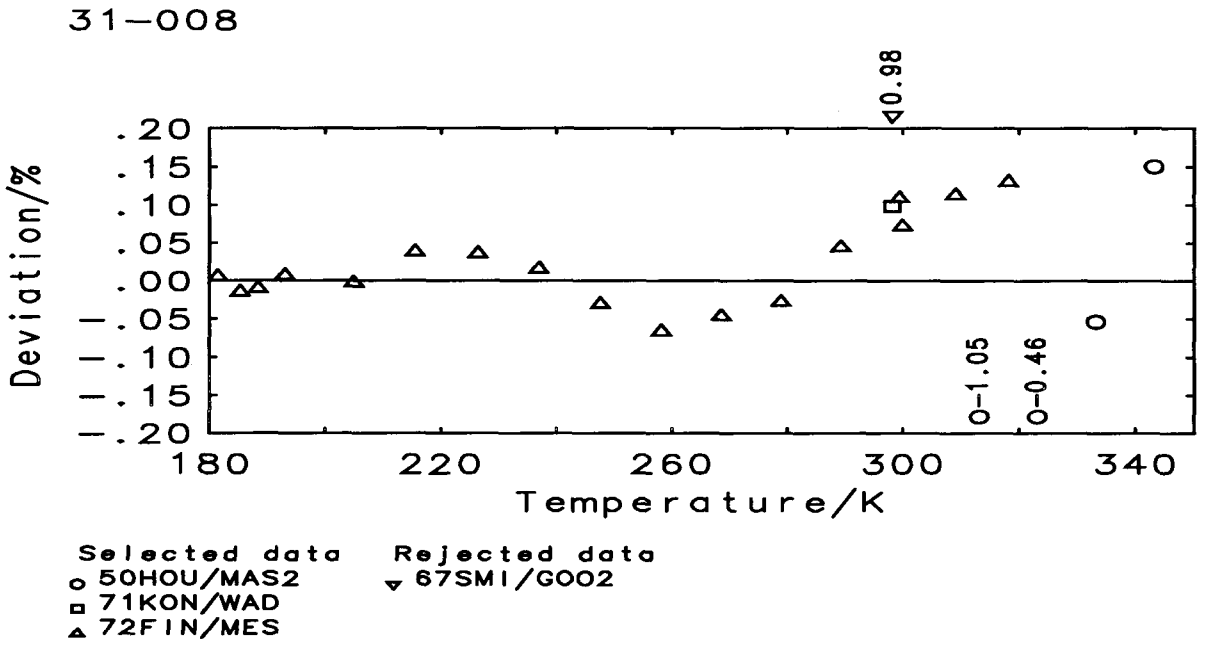
TABLE 31.8.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1} g^{-1}$)	2.484	2.530	2.570	2.603	2.632	2.656	2.676
C_p ($J K^{-1} mol^{-1}$)	146.8	149.6	151.9	153.9	155.6	157.0	158.2
c_{sat} ($J K^{-1} g^{-1}$)	2.484	2.530	2.570	2.603	2.632	2.656	2.676
C_{sat} ($J K^{-1} mol^{-1}$)	146.8	149.6	151.9	153.9	155.6	157.0	158.2
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	2.694	2.710	2.726	2.730	2.741	2.757	2.772
C_p ($J K^{-1} mol^{-1}$)	159.2	160.2	161.1	161.4	162.0	163.0	163.8
c_{sat} ($J K^{-1} g^{-1}$)	2.694	2.710	2.725	2.730	2.740	2.756	2.770
C_{sat} ($J K^{-1} mol^{-1}$)	159.3	160.2	161.1	161.4	162.0	162.9	163.7
Temp. (K)	300	310	320	330	340		
c_p ($J K^{-1} g^{-1}$)	2.775	2.796	2.820	2.849	2.883		
C_p ($J K^{-1} mol^{-1}$)	164.0	165.3	166.7	168.4	170.4		
c_{sat} ($J K^{-1} g^{-1}$)	2.773	2.792	2.815	2.842	2.874		
C_{sat} ($J K^{-1} mol^{-1}$)	163.9	165.1	166.4	168.0	169.9		

TABLE 31.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	23	0.815	4.85–2	0.25	–6.57–4	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
181.5–343.1	471.80	1.88264+2	2.15811+1	–2.78192+1	3.01046+2	–1.88991+2	2.46773+2	III



Name: (*R*,*S*)–1,2–Propanediamine
Formula: $C_3H_{10}N_2$

CAS–RN: 10424–38–1
Group No.: 31–009
Molar Mass: 74.13

TABLE 31.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75MES/FIN	240.0–367.6	17	0.20	99.67	melpt	C_{sat}	BSAO	47HUF

TABLE 31.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.163	8.05–3	0.03	3.59–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
240.0–367.6		2.03397+1	3.52390	–1.25642	1.90115–1		II

TABLE 31.9.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	2.713	2.722	2.731	2.741	2.744	2.751	2.763
C_{sat} (J K^{-1}mol^{-1})	201.1	201.8	202.5	203.2	203.4	204.0	204.8
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	2.772	2.775	2.788	2.802	2.817	2.834	2.853
C_{sat} (J K^{-1}mol^{-1})	205.5	205.7	206.6	207.7	208.8	210.1	211.5
Temp. (K)	360	370					
c_{sat} (J K^{-1}g^{-1})	2.873	2.895					
C_{sat} (J K^{-1}mol^{-1})	213.0	214.6					

TABLE 31.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.169	8.31–3	0.03	5.05–6	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
240.0–367.6	607.00	1.52393	2.46074	2.07943+1	2.35940–1		II

Name: 1–Butanamine
Formula: $C_4H_{11}N$

CAS–RN: 109–73–9
Group No.: 31–010
Molar Mass: 73.14

TABLE 31.10.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71KON/WAD	298.15	2.570	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: *N*–Ethylethanamine
Formula: $C_4H_{11}N$

CAS–RN: 109–89–7
Group No.: 31–011
Molar Mass: 73.14

TABLE 31.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
65KAU/BIT		293.1–323.1	4S	1.00	not specified		C_p	FSIO	65KAU/BIT
85COS/PAT9		283.1–313.1	3S	nosp	99.5	chrom	C_p	FSIT	71PIC/LED

36KUR/VOS average value in temperature range 290–333 K

TABLE 31.11.2. Correlated heat capacities

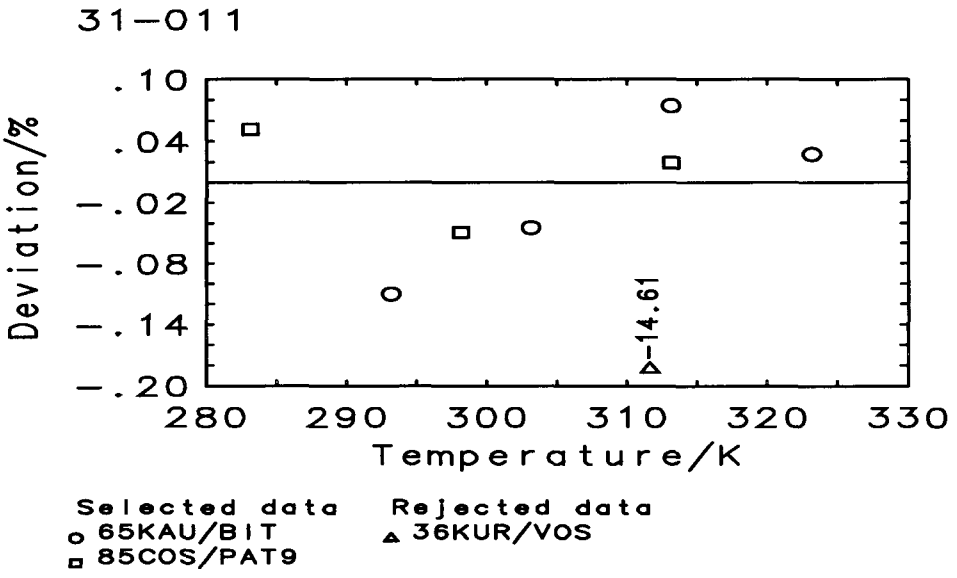
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65KAU/BIT	293.1–323.1	4	1.00	0.072	1.54–2	0.07	–3.13–3	0
85COS/PAT9	283.1–313.1	3	0.50#	0.085	8.98–3	0.04	1.06–3	1
				Rejected data				
36KUR/VOS	(2.79, 14.62, –2.79, –1)							

TABLE 31.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.092	1.55–2	0.07	–1.33–3	1
Temp. range K		A_1	A_2				Level of uncertainty
283.1–323.1		1.21624+1	3.10881				IV

TABLE 31.11.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.372	2.408	2.436	2.443	2.478	2.514
C_p (J K^{-1}mol^{-1})	173.5	176.1	178.2	178.7	181.3	183.8



Name: 2–Methyl–1–propanamine
Formula: $C_4H_{11}N$

CAS–RN: 78–81–9
Group No.: 31–012
Molar Mass: 73.14

TABLE 31.12.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.15	2.653	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: 2–Methyl–2–propanamine
Formula: $C_4H_{11}N$

CAS–RN: 75–64–9
Group No.: 31–013
Molar Mass: 73.14

TABLE 31.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67SMI/GOO2	298.1	1	nosp	99.990	melpt	C_p	not specified	
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM
72FIN/MES	209.8–332.5	20	0.20	99.993	melpt	C_{sat}	BSAO	47HUF

TABLE 31.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67SMI/GOO2	298.1	1	0.30#	0.049	3.42–3	0.01	3.42–3	1
72FIN/MES	209.8–332.5	20	0.20	0.073	3.40–3	0.01	–7.50–5	–2
				Rejected data				
71KON/WAD	(2.21–1, 0.97,–2.21–1, –1)							

TABLE 31.13.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	21	0.083	3.89–3	0.02	9.14–5	–1
C_{sat}	22	21	0.083	3.87–3	0.02	6.26–5	–1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
209.8–270.0	–3.03111+1	5.74378+1	–2.12498+1	2.68171	II
270.0–332.5	9.27248	1.34560+1	–4.96026	6.70652–1	II
209.8–270.0	–2.92438+1	5.60902+1	–2.06852+1	2.60323	II
270.0–332.5	9.02007	1.35748+1	–4.93878	6.59227–1	II

TABLE 31.13.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J\,K^{-1}g^{-1}$)	2.436	2.473	2.502	2.525	2.544	2.559	2.574
C_p ($J\,K^{-1}mol^{-1}$)	178.2	180.9	183.0	184.7	186.0	187.2	188.3
c_{sat} ($J\,K^{-1}g^{-1}$)	2.436	2.473	2.502	2.525	2.544	2.559	2.574
C_{sat} ($J\,K^{-1}mol^{-1}$)	178.2	180.9	183.0	184.7	186.0	187.2	188.3
Temp. (K)	**273.15**	**280**	**290**	**298.15**	**300**	**310**	**320**
c_p ($J\,K^{-1}g^{-1}$)	2.579	2.590	2.607	2.623	2.627	2.649	2.673
C_p ($J\,K^{-1}mol^{-1}$)	188.6	189.4	190.7	191.8	192.1	193.7	195.5
c_{sat} ($J\,K^{-1}g^{-1}$)	2.579	2.590	2.607	2.622	2.625	2.646	2.670
C_{sat} ($J\,K^{-1}mol^{-1}$)	188.6	189.4	190.6	191.8	192.0	193.6	195.3
Temp. (K)	**330**						
c_p ($J\,K^{-1}g^{-1}$)	2.701						
C_p ($J\,K^{-1}mol^{-1}$)	197.6						
c_{sat} ($J\,K^{-1}g^{-1}$)	2.697						
C_{sat} ($J\,K^{-1}mol^{-1}$)	197.3						

TABLE 31.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	21	0.463	2.10–2	0.09	–7.67–4	1
Temp. range K	**T_c K**	**A_1**	**A_2**	**A_3**	**A_4**	**A_5**	**A_6**	**Level of uncertainty**
209.8–332.5	483.90	4.12417+2	4.76717+1	–6.63260+1	5.94216+2	–3.14170+2	4.84118+2	II

Name: 2–Methyl–1,2–propanediamine
Formula: $C_4H_{12}N_2$

CAS–RN: 811–93–8
Group No.: 31–014
Molar Mass: 88.15

TABLE 31.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75MES/FIN	257.7–374.6	17	0.20	99.37	melpt	C_{sat}	BSAO	47HUF

TABLE 31.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	17	17	0.558	3.15–2	0.11	5.78–5	–5
Temp. range K		**A_1**	**A_2**	**A_3**			**Level of uncertainty**
257.7–374.6		2.86600+1	–1.72754	5.30623–1			II

TABLE 31.14.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	2.618	2.628	2.632	2.639	2.652	2.662	2.665
C_{sat} (J K^{-1}mol^{-1})	230.8	231.7	232.0	232.7	233.7	234.7	234.9
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	2.679	2.694	2.711	2.728	2.746	2.765	2.785
C_{sat} (J K^{-1}mol^{-1})	236.2	237.5	238.9	240.5	242.1	243.8	245.5

Name: *N*–(2–Aminoethyl)–1,2–ethanediamine
Formula: $C_4H_{13}N_3$

CAS–RN: 111–40–0
Group No.: 31–015
Molar Mass: 103.17

TABLE 31.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	313.1–493.1	10	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 31.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.141	2.85–1	0.85	2.89–3	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
313.1–493.1		1.71327+2	–1.10577+2	2.79863+1	–2.24057		VI

TABLE 31.15.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	2.48	2.47	2.47	2.48	2.50	2.53	2.57
C_{sat} (J K^{-1}mol^{-1})	256	255	255	256	258	261	265
Temp. (K)	380	390	400	410	420	430	440
c_{sat} (J K^{-1}g^{-1})	2.60	2.65	2.69	2.74	2.79	2.83	2.88
C_{sat} (J K^{-1}mol^{-1})	269	273	278	283	288	292	297
Temp. (K)	450	460	470	480	490		
c_{sat} (J K^{-1}g^{-1})	2.92	2.96	3.00	3.03	3.05		
C_{sat} (J K^{-1}mol^{-1})	302	306	309	312	315		

TABLE 31.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.247	4.98–1	1.48	1.03–2	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
313.1–493.1	678.00	–5.99016	1.10264	2.06389+1	8.13548		VI

Name: Cyclopentanamine
Formula: $C_5H_{11}N$

CAS–RN: 1003–03–8
Group No.: 31–016
Molar Mass: 85.15

TABLE 31.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81FIN/MES	197.0–348.7	15	0.20	99.916	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 31.16.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.244	1.04–2	0.05	6.74–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
197.0–280.0		4.21088	1.74115+1	–6.50109	8.85460–1		II
280.0–348.7		2.48027+1	–4.65121	1.37845	–5.25799–2		II

TABLE 31.16.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.964	1.983	2.000	2.015	2.030	2.045	2.060
C_{sat} (J K^{-1}mol^{-1})	167.2	168.8	170.3	171.6	172.9	174.1	175.4
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.076	2.081	2.093	2.112	2.128	2.132	2.155
C_{sat} (J K^{-1}mol^{-1})	176.7	177.2	178.2	179.8	181.2	181.6	183.5
Temp. (K)	320	330	340	350			
c_{sat} (J K^{-1}g^{-1})	2.179	2.204	2.232	2.261			
C_{sat} (J K^{-1}mol^{-1})	185.5	187.7	190.0	192.5			

TABLE 31.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	15	0.877	3.66–2	0.18	1.04–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
196.9–348.7	582.00	–2.09490	1.78894	1.63400+1	6.13295–1		II

Name: *N*–Ethyl–*N*–methylethanamine
Formula: $C_5H_{13}N$

CAS–RN: 616–39–7
Group No.: 31–017
Molar Mass: 87.16

TABLE 31.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80ROU/ROB	283.1–313.1	3	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 31.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	7.040	5.01–1	2.11	1.40–2	–1

Temp. range K	A_1	Level of uncertainty
283.1–313.1	2.34790+1	V

TABLE 31.17.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	2.24	2.24	2.24	2.24	2.24
C_p ($J K^{-1}mol^{-1}$)	195	195	195	195	195

Name: 1–Pentanamine
Formula: $C_5H_{13}N$

CAS–RN: 110–58–7
Group No.: 31–018
Molar Mass: 87.16

TABLE 31.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
01KAH	N	329.1	1	nosp	not specified		C_{avg}	DSIO	01KAH
71KON/WAD		298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

01KAH average value in temperature range 294–364 K

TABLE 31.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
01KAH	329.1	1		5.00#	0.000	0.00	0.00	0.000
71KON/WAD	298.1	1		0.50#	0.000	0.00	0.00	0.000

TABLE 31.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–329.1		1.95346+1	2.24203				IV

TABLE 31.18.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	2.484	2.501	2.505	2.526	2.548	2.569
C_p ($J K^{-1} mol^{-1}$)	216.5	218.0	218.3	220.2	222.1	223.9

Name: *N,N*–Dimethyl–1,3–propanediamine
Formula: $C_5H_{14}N_2$

CAS–RN: 109–55–7
Group No.: 31–019
Molar Mass: 102.18

TABLE 31.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
82DZH/KAR2		194.4–300.0	12S	0.20	not specified		C_p	BSAO	54STR/ICK
84LEB/GUT	N	295.6–358.6	5	0.30	99.9	chrom	C_p	BSAO	76LEB/LIT

84LEB/GUT same data in 81LEB/RYA

TABLE 31.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82DZH/KAR2	194.4–300.0	12	0.20	1.099	6.67–2	0.22	3.51–2	3
84LEB/GUT	295.6–358.6	5	0.30	3.960	3.63–1	1.19	–1.79–1	–1

TABLE 31.19.3. Parameters of regression polynomial

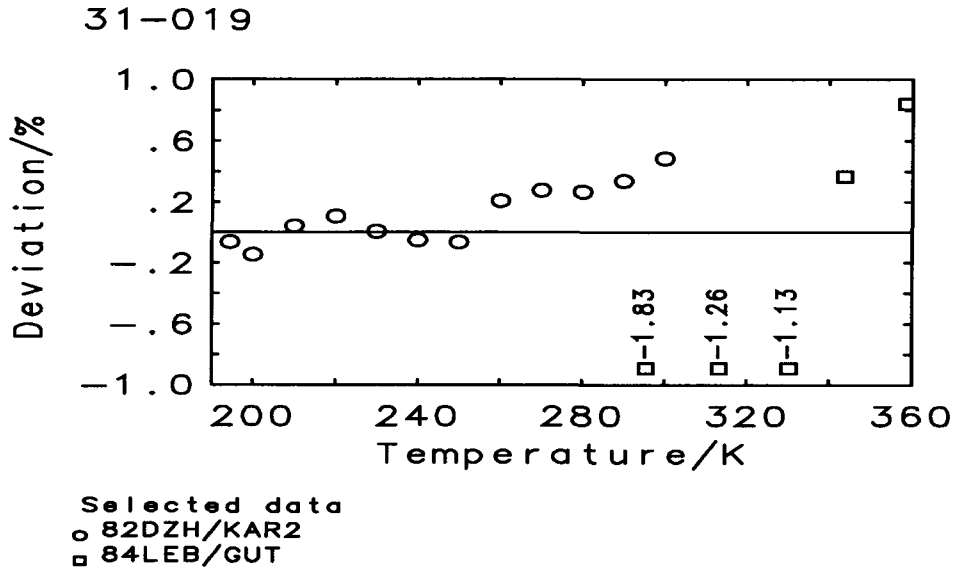
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	2.576	2.26–1	0.74	–2.79–2	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
194.4–358.6		2.83502+1	–9.73429–1	5.74965–1			V

TABLE 31.19.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1} g^{-1}$)	2.34	2.35	2.36	2.37	2.39	2.40	2.42
C_p ($J K^{-1} mol^{-1}$)	239	240	241	242	244	245	247
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	2.43	2.44	2.45	2.47	2.49	2.49	2.51
C_p ($J K^{-1} mol^{-1}$)	249	249	251	252	254	254	257
Temp. (K)	320	330	340	350	360		
c_p ($J K^{-1} g^{-1}$)	2.53	2.56	2.58	2.60	2.63		
C_p ($J K^{-1} mol^{-1}$)	259	261	263	266	269		

TABLE 31.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	2.565	2.07–1	0.68	–6.43–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
194.4–358.6	588.00	9.02954–2	3.47672	2.34885+1	5.86276–4		V



Name: Benzenamine
Formula: C_6H_7N

CAS–RN: 62–53–3
Group No.: 31–020
Molar Mass: 93.13

TABLE 31.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
28LAN	N	274.2–332.0	14	nosp	not specified	C_p	FSIO	28LAN
31BLA/LEI		303.1–412.8	22	3.00	not specified	C_{sat}	BSIO	31BLA/LEI
33FER/MIL		291.6–322.8	12	1.00	not specified	C_{sat}	BDHO	33FER/MIL
33PAR/HUF		275.7–298.2	3	1.00	not specified	C_p	BSIO	25PAR
34RAD/JUL		288.1	1	nosp	not specified	C_p	BSIO	49WEI
37ELL		298.1–351.1	3S	nosp	not specified	C_p	BSIO	37ELL
50HOU/MAS2		323.1–453.1	10S	0.40	not specified	C_p	BSAO	50SAG/HOU
57CRU/JOS		293.1	1	2.00	not specified	C_p	BSIO	57CRU/JOS
62HAT/HIL		270.2–313.1	17	nosp	99.98 melpt	C_p	BSAO	58HIL/KRA
71DES/BHA		298.1–318.1	3S	1.00	not specified	C_p	BSIO	56MUR/VAN
75NIC/WAD		298.1	1	nosp	99.5 chrom	C_p	BSIO	70LKB/COM
87LES/LIC		270.0–310.0	eqn	2.00	99. estim	C_p	BDHT	69PER/COM
90RAO/RAJ		318.1–333.1	4	4.00	not specified	C_p	BDHT	89PRA/RAJ

28LAN corrected for water content (about 0.1 mass %)

TABLE 31.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50HOU/MAS2	323.1–453.1	10	0.40	0.413	3.93–2	0.17	1.60–2	2
62HAT/HIL	270.2–313.1	17	0.30#	0.612	4.22–2	0.18	–4.08–3	–3
75NIC/WAD	298.1	1	0.50#	0.420	4.83–2	0.21	–4.83–2	–1
				Rejected data				
28LAN	(2.37–1, 1.02, 1.63–1, 10)			31BLA/LEI	(1.84, 6.33, 1.30, 22)			
33FER/MIL	(1.99–1, 0.86, 1.89–1, 12)			33PAR/HUF	(1.16–1, 0.51, –1.03–1, –3)			
34RAD/JUL	(7.09–1, 3.21,–7.09–1, –1)			37ELL	(3.29–1, 1.35, 2.90–1, 3)			
57CRU/JOS	(1.87–1, 0.81, 1.87–1, 1)			71DES/BHA	(4.52–1, 1.89, 4.34–1, 3)			
87LES/LIC	(3.23+3, 100.70, –3.23+3, 3)			90RAO/RAJ	(1.21, 4.65, 7.70–1, 2)			

TABLE 31.20.3. Parameters of cubic spline polynomials

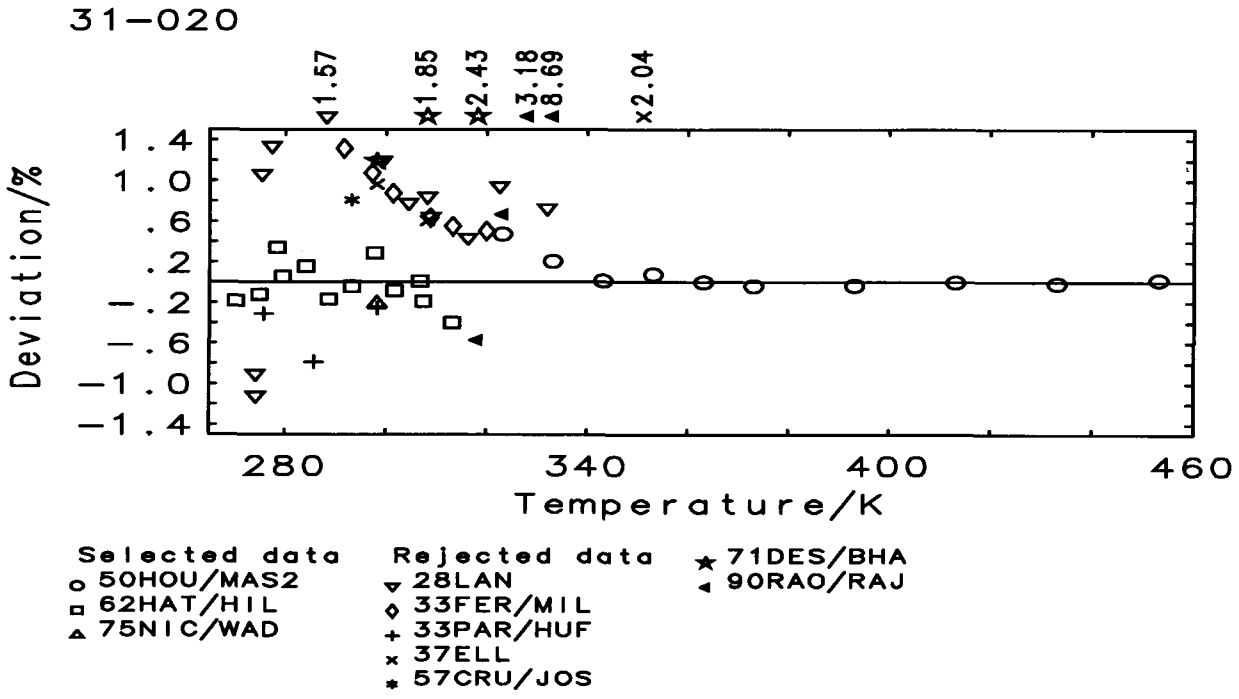
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	95	28	0.599	4.57–2	0.20	1.52–3	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
270.2–330.0		9.68899+1	–7.44027+1	2.42128+1	–2.53824		II
330.0–453.1		–9.76973	2.25606+1	–5.17006	4.29719–1		IV

TABLE 31.20.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	2.014	2.016	2.024	2.040	2.055	2.059	2.081
C_p ($J K^{-1} mol^{-1}$)	187.5	187.8	188.5	190.0	191.4	191.8	193.8
Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1} g^{-1}$)	2.104	2.127	2.148	2.168	2.187	2.205	2.222
C_p ($J K^{-1} mol^{-1}$)	195.9	198.1	200.0	201.9	203.7	205.3	206.9
Temp. (K)	390	400	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	2.238	2.255	2.271	2.288	2.305	2.322	2.341
C_p ($J K^{-1} mol^{-1}$)	208.5	210.0	211.5	213.0	214.6	216.3	218.0

TABLE 31.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	95	28	0.951	7.18–2	0.31	7.48–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
270.2–453.1	699.00	5.46607	2.99934–1	1.49619+1	2.49038+1		IV



Name: 1,3–Benzenediamine
Formula: $C_6H_8N_2$

CAS–RN: 108–45–2
Group No.: 31–021
Molar Mass: 108.14

TABLE 31.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84RAB/KAR		342.4–451.4	22	1.50	99.44	melpt	C_p	BSAO	76LEB/LIT
87LES/LIC	N	270.0–370.0	eqn	2.00	99.	estim	C_p	BDHT	69PER/COM

87LES/LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 31.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
84RAB/KAR	342.4–451.4	22	1.50	0.415	1.86–1	0.62	2.34–3	0
				Rejected data				
87LES/LIC	(3.13, 11.95, –3.13, –3)							

TABLE 31.21.3. Parameters of regression polynomial

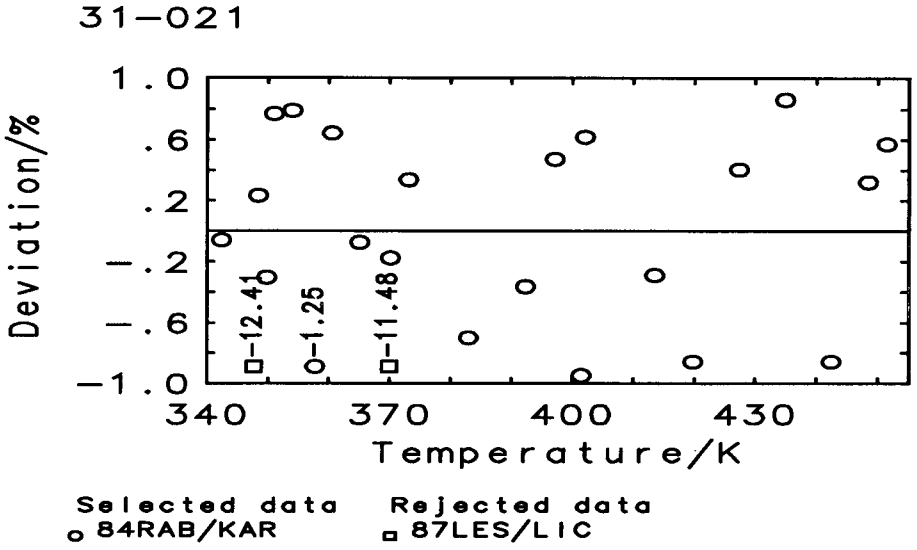
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	22	0.435	1.95–1	0.65	2.34–3	0
Temp. range K		A_1	A_2				Level of uncertainty
342.4–451.4		2.30074+1	1.77242				V

TABLE 31.21.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1} g^{-1}$)	2.23	2.25	2.26	2.27	2.29	2.30	2.31
C_p ($J K^{-1} mol^{-1}$)	241	243	244	246	247	249	250

TABLE 31.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	22	0.433	1.94–1	0.65	2.18–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
342.4–451.4	815.00	1.21528	4.38291	2.22114+1	8.42424–2		V



Name: Cyclohexanamine
Formula: $C_6H_{13}N$

CAS-RN: 108–91–8
Group No.: 31–022
Molar Mass: 99.18

TABLE 31.22.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79STE	N	298.15	3.570	nosp	not specified		C_p	not specified	

79STE the origin of data unclear; 0.05 mol.% water was detected

Name: *N,N*–Diethylethanamine
Formula: $C_6H_{15}N$

CAS-RN: 121–44–8
Group No.: 31–023
Molar Mass: 101.19

TABLE 31.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	319.7–330.0	3S	nosp	not specified		C_{avg}	DSIO	*81VON
65KAU/BIT	293.1–343.1	6	1.00	not specified		C_p	FSIO	65KAU/BIT
80ROU/ROB	278.1–288.1	2	0.30	not specified		C_p	FSIT	71PIC/LED
85HEP/KOO	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
91GRO/ROU	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED

TABLE 31.23.2. Correlated heat capacities

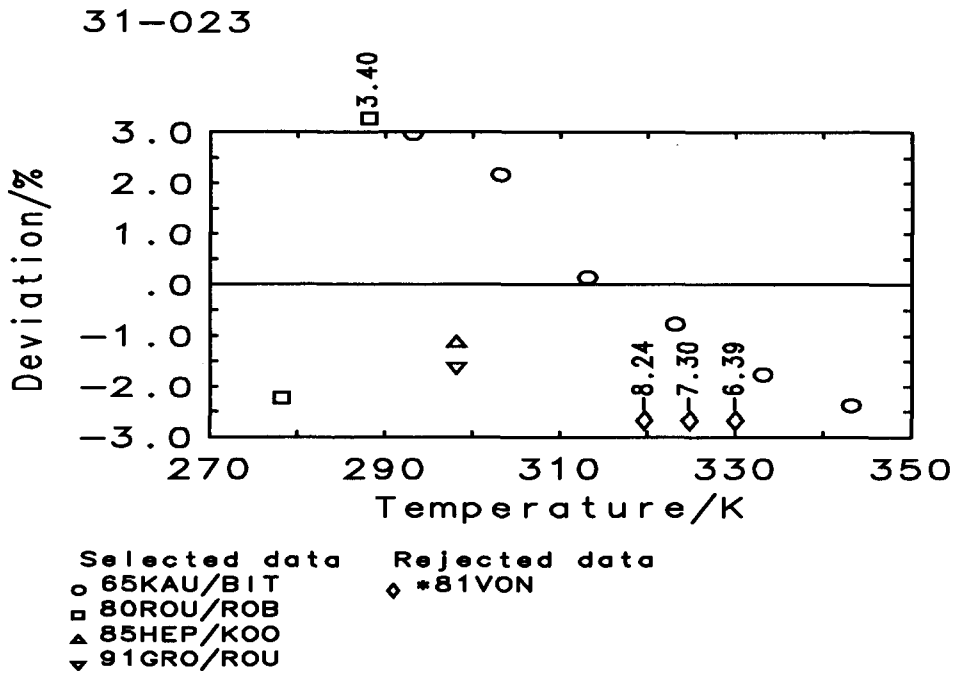
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65KAU/BIT	293.1–343.1	6	1.00	1.954	5.52–1	1.95	–3.85–3	0
80ROU/ROB	278.1–288.1	2	0.30	9.580	7.40–1	2.87	1.80–1	0
85HEP/KOO	298.1	1	0.50#	2.287	3.00–1	1.14	–3.00–1	–1
91GRO/ROU	298.1	1	0.50#	3.219	4.20–1	1.61	–4.20–1	–1
				Rejected data				
*81VON	(1.99, 7.35,–1.98, –3)							

TABLE 31.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	10	5.268	6.32–1	2.33	–3.83–2	–2
Temp. range K		A_1	A_2				Level of uncertainty
278.1–343.1		–2.37412	9.69488				V

TABLE 31.23.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.04	2.12	2.18	2.19	2.27	2.35	2.43
C_p (J K^{-1}mol^{-1})	206	214	221	222	230	238	246
Temp. (K)	340						
c_p (J K^{-1}g^{-1})	2.51						
C_p (J K^{-1}mol^{-1})	254						



Name: 1–Hexanamine
Formula: $C_6H_{15}N$

CAS–RN: 111–26–2
Group No.: 31–024
Molar Mass: 101.19

TABLE 31.24.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.15	2.490	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: *N*–Propyl–1–propanamine
Formula: $C_6H_{15}N$

CAS–RN: 142–84–7
Group No.: 31–025
Molar Mass: 101.19

TABLE 31.25.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
01KAH	N	334.15	2.499	nosp	not specified		C_{avg}	DSIO	01KAH

01KAH average value in temperture range 294–374 K

Name: *N,N'*–Bis(2–aminoethyl)–1,2–ethanediamine
Formula: $C_6H_{18}N_4$

CAS–RN: 112–24–3
Group No.: 31–026
Molar Mass: 146.24

TABLE 31.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	333.1–473.1	8	6.00	97.	chrom	C_p	BDCT	86MER/BEN

TABLE 31.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.119	3.47–1	0.72	3.13–3	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
333.1–473.1		5.40923+1	–7.44475	1.45213			VI

TABLE 31.26.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p (J K^{-1}g^{-1})	2.58	2.59	2.61	2.62	2.64	2.66	2.68
C_p (J K^{-1}mol^{-1})	377	379	381	383	386	389	392
Temp. (K)	400	410	420	430	440	450	460
c_p (J K^{-1}g^{-1})	2.70	2.73	2.75	2.78	2.81	2.84	2.88
C_p (J K^{-1}mol^{-1})	395	399	403	407	411	416	420
Temp. (K)	470						
c_p (J K^{-1}g^{-1})	2.91						
C_p (J K^{-1}mol^{-1})	426						

TABLE 31.26.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.117	3.43–1	0.70	3.01–3	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
333.1–473.1	717.00	2.12338	6.51097	3.44613+1	1.73121–1	VI

Name: Benzenemethanamine
Formula: C_7H_9N

CAS–RN: 100–46–9
Group No.: 31–027
Molar Mass: 107.16

TABLE 31.27.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75NIC/WAD	298.15	1.933	nosp	99.5	chrom	C_p	BSIO	70LKB/COM

Name: *N*–Methylbenzenamine
Formula: C_7H_9N

CAS–RN: 100–61–8
Group No.: 31–028
Molar Mass: 107.16

TABLE 31.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
02LOU2	N	378.8	1	nosp	not specified		C_{avg}	DSIO	*98LOU
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
57CRU/JOS		293.1–338.1	2	2.00	not specified		C_p	BSIO	57CRU/JOS
87LES/LIC		240.0–330.0	eqn	2.00	99.	estim	C_p	BDHT	69PER/COM

02LOU2 average value in temperature range 294–464 K
36KUR/VOS average value in temperature range 290–333 K

TABLE 31.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
02LOU2	378.8	1	5.00#	0.039	5.36–2	0.19	–5.36–2	–1
57CRU/JOS	293.1–338.1	2	2.00	0.294	1.49–1	0.59	1.44–1	2
87LES/LIC	240.0–330.0	10	2.00	0.069	3.51–2	0.14	–2.75–2	–7
				Rejected data				
36KUR/VOS	(2.25, 8.15, 2.25, 1)							

TABLE 31.28.3. Parameters of regression polynomial

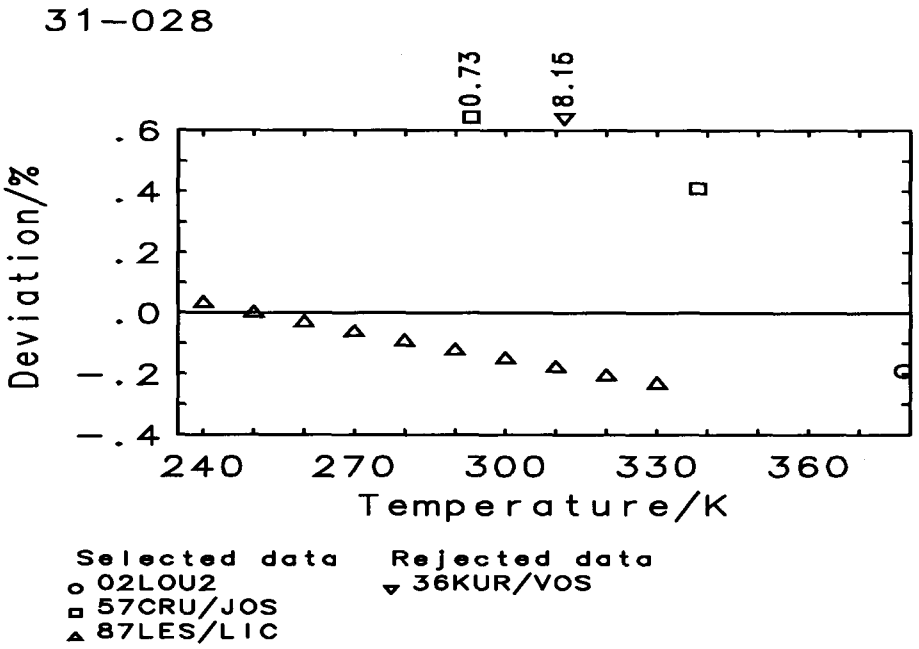
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	0.142	7.35–2	0.29	–3.12–3	–6
Temp. range K		A_1	A_2				Level of uncertainty
240.0–378.8		1.47980+1	3.40473				V

TABLE 31.28.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J\,K^{-1}g^{-1}$)	1.78	1.81	1.84	1.86	1.87	1.89	1.91
C_p ($J\,K^{-1}mol^{-1}$)	191	194	197	199	200	202	205
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.94	1.94	1.97	1.99	2.02	2.05	2.07
C_p ($J\,K^{-1}mol^{-1}$)	207	208	211	214	216	219.	222
Temp. (K)	360	370	380				
c_p ($J\,K^{-1}g^{-1}$)	2.10	2.13	2.15				
C_p ($J\,K^{-1}mol^{-1}$)	225	228	231				

TABLE 31.28.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	0.150	7.60–2	0.30	1.43–3	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
240.0–378.8	715.00	2.10278	3.97507–2	1.44231+1	2.78088+1		V



Name: 2–Methylbenzenamine
Formula: C_7H_9N

CAS–RN: 95–53–4
Group No.: 31–029
Molar Mass: 107.16

TABLE 31.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON		330.8–392.2	4S	nosp	not specified	C_{avg}	DSIO	*81VON
*87SCH	N	320.3–348.5	6S	nosp	not specified	C_p	DSIO	*86SCH
02LOU2	N	381.0–382.0	2	nosp	not specified	C_{avg}	DSIO	*98LOU
34KOL/UDO2	N	302.5	1	nosp	not specified	C_p	BSIT	34KOL/UDO2
34RAD/JUL		288.1	1	nosp	not specified	C_p	BSIO	49WEI
88GUS/MIR		303.1–463.1	9	1.90	not specified	C_p	BDHT	84GUS/MIR
90MEV/LIC		249.5	1	3.00	99. anal	C_p	BDCT	89BRE/LIC

*87SCH two data points near the upper temperature limit are misprinted; corrected to comply with equation presented by the author
02LOU2 average value in temperature range 295–468 K
34KOL/UDO2 same datum in 34KOL/UDO1

TABLE 31.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	330.8–392.2	4	2.00#	0.773	4.19–1	1.55	–3.76–1	–4
*87SCH	320.3–348.5	6	2.00#	0.685	3.85–1	1.37	3.21–1	6
02LOU2	381.0–382.0	2	5.00#	0.135	1.89–1	0.67	–1.49–1	–2
90MEV/LIC	249.6	1	3.00	0.746	5.62–1	2.24	–5.62–1	–1
				Rejected data				
34KOL/UDO2	(1.55, 6.14,–1.55, –1)			34RAD/JUL	(2.19, 9.03,–2.19, –1)			
88GUS/MIR	(6.73, 32.42, –6.72, –5)							

TABLE 31.29.3. Parameters of regression polynomial

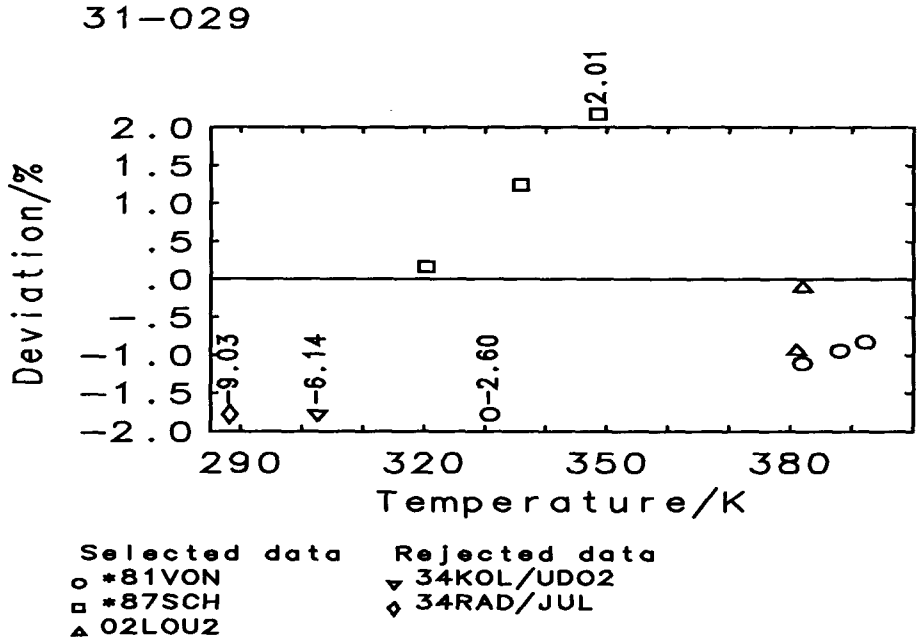
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	13	0.726	4.24–1	1.56	–3.37–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
249.6–392.2		2.07229+1	1.99414				V

TABLE 31.29.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.99	2.01	2.03	2.03	2.04	2.06	2.07
C_p (J K^{-1}mol^{-1})	214	215	217	218	219	220	222
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.07	2.09	2.10	2.12	2.13	2.15	2.16
C_p (J K^{-1}mol^{-1})	222	224	225	227	229	230	232
Temp. (K)	370	380	390				
c_p (J K^{-1}g^{-1})	2.18	2.20	2.21				
C_p (J K^{-1}mol^{-1})	234	235	237				

TABLE 31.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	13	0.649	3.57–1	1.31	–2.71–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
249.6–392.2	694.00	9.57702+1	1.69943+1	–7.29132	1.34927+2		V



Name: 3–Methylbenzenamine
Formula: C_7H_9N

CAS–RN: 108–44–1
Group No.: 31–030
Molar Mass: 107.16

TABLE 31.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
34KOL/UDO2	N	302.7	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
88GUS/MIR		303.1–463.1	9	1.90	not specified		C_p	BDHT	84GUS/MIR
90MEV/LIC		241.6	1	3.00	99.	anal	C_p	BDCT	89BRE/LIC

34KOL/UDO2 same datum in 34KOL/UDO1

TABLE 31.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
34KOL/UDO2	302.7	1	5.00#	0.000	0.00	0.00	0.00	0
90MEV/LIC	241.6	1	3.00	0.000	0.00	0.00	0.00	0

TABLE 31.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
241.6–302.7		2.01816+1	1.95103				VI

TABLE 31.30.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.94	1.96	1.97	1.98	1.99	2.00	2.02
C_p (J K^{-1}mol^{-1})	208	210	212	212	213	215	216
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	2.02						
C_p (J K^{-1}mol^{-1})	216						

Name: 4–Methylbenzenamine
Formula: C_7H_9N

CAS–RN: 106–49–0
Group No.: 31–031
Molar Mass: 107.16

TABLE 31.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90MEV/LIC	323.0–368.0	eqn	3.00	99.	anal	C_p	BDCT	89BRE/LIC

TABLE 31.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	1.91–6	0.00	–3.82–7	0
Temp. range K		A_1	A_2				Level of uncertainty
323.0–368.2		1.96366+1	2.18895				V

TABLE 31.31.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.07	2.08	2.10	2.12	2.14	2.15
C_p (J K^{-1}mol^{-1})	222	223	225	227	229	231

Name: Benzeneethanamine
Formula: $C_8H_{11}N$

CAS–RN: 64–04–0
Group No.: 31–032
Molar Mass: 121.18

TABLE 31.32.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75NIC/WAD	298.15	1.974	nosp	99.5	chrom	C_p	BSIO	70LKB/COM

Name: *N,N*–Dimethylbenzenamine
Formula: $C_8H_{11}N$

CAS–RN: 121–69–7
Group No.: 31–033
Molar Mass: 121.18

TABLE 31.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		329.5–388.1	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*87SCH		318.0–348.3	6S	nosp	not specified		C_p	DSIO	*86SCH
02LOU2	N	376.8–378.0	2	nosp	not specified		C_{avg}	DSIO	*98LOU
16BRA		283.1	1	nosp	not specified		C_{avg}	DSTO	16BRA
34KOL/UDO2	N	302.3	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
34RAD/JUL		289.1	1	nosp	not specified		C_p	BSIO	49WEI
57CRU/JOS		293.1	1	2.00	not specified		C_p	BSIO	57CRU/JOS

02LOU2 average value in temperature range 294–459 K
34KOL/UDO2 same datum in 34KOL/UDO1

TABLE 31.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	329.5–388.1	4	2.00#	0.490	2.81–1	0.98	–2.80–1	–4
*87SCH	318.0–348.3	6	2.00#	0.587	3.35–1	1.17	2.58–1	2
02LOU2	376.8–378.0	2	3.00#	0.050	4.38–2	0.15	8.01–3	0
16BRA	283.1	1	3.00#	0.215	1.64–1	0.64	–1.64–1	–1
57CRU/JOS	293.1	1	2.00	0.556	2.87–1	1.11	–2.87–1	–1
				Rejected data				
34KOL/UDO2	(6.04–1, 2.34,–6.04–1, –1)			34RAD/JUL	(6.65–1, 2.63, –6.65–1, –1)			

TABLE 31.33.3. Parameters of regression polynomial

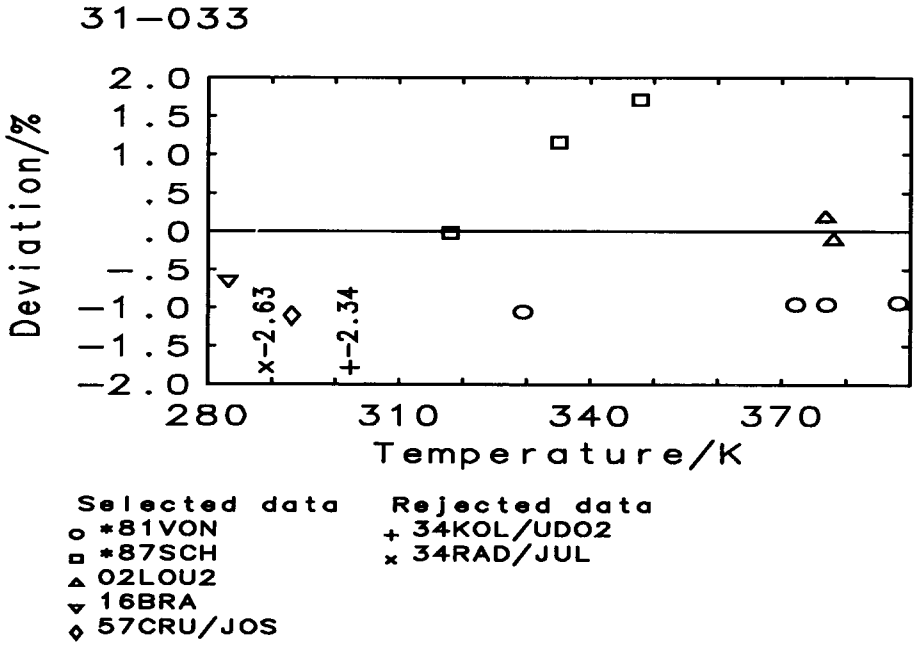
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	14	0.532	3.03–1	1.07	–7.41–4	–4
Temp. range K		A_1	A_2				Level of uncertainty
283.1–388.1		1.44131+1	3.97001				V

TABLE 31.33.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.75	1.78	1.80	1.81	1.83	1.86	1.89
C_p ($J K^{-1} mol^{-1}$)	212	216	218	219	222	225	229
Temp. (K)	340	350	360	370	380	390	
c_p ($J K^{-1} g^{-1}$)	1.92	1.94	1.97	2.00	2.02	2.05	
C_p ($J K^{-1} mol^{-1}$)	232	235	239	242	245	249	

TABLE 31.33.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	14	0.428	2.45–1	0.88	–1.53–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
283.1–388.1	687.00	1.09226+2	1.68339+1	–1.83199+1	1.77177+2		V



Name: 2,6–Dimethylbenzenamine
Formula: $C_8H_{11}N$

CAS–RN: 87–62–7
Group No.: 31–034
Molar Mass: 121.18

TABLE 31.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86STE/CHI	284.6–450.0	19S	nosp	99.99	melpt	C_{sat}	BSAO	47HUF

TABLE 31.34.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.126	3.99–3	0.01	5.02–7	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
284.6–370.0		2.41023+1	–1.19416	1.16300	–8.10198–2		II
370.0–450.0		3.21548+1	–7.72325	2.92762	–2.39995–1		II

TABLE 31.34.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.952	1.971	1.976	2.001	2.026	2.053	2.079
C_{sat} (J K^{-1}mol^{-1})	236.5	238.9	239.5	242.5	245.6	248.7	251.9
Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	2.106	2.134	2.161	2.190	2.218	2.247	2.275
C_{sat} (J K^{-1}mol^{-1})	255.2	258.5	261.9	265.3	268.8	272.3	275.7
Temp. (K)	420	430	440	450			
c_{sat} (J K^{-1}g^{-1})	2.304	2.332	2.361	2.389			
C_{sat} (J K^{-1}mol^{-1})	279.2	282.7	286.1	289.5			

TABLE 31.34.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.692	2.20–2	0.07	2.87–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
284.6–450.0	712.00	–4.07741	2.19186–1	1.82017+1	1.89625+1		II

Name: 2–Methyl–*N*–(2–methylpropyl)–1–propanamine
Formula: $C_8H_{19}N$

CAS–RN: 110–96–3
Group No.: 31–035
Molar Mass: 129.25

TABLE 31.35.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
01KAH	N	349.15	2.387	nosp	not specified		C_{avg}	DSIO	01KAH

01KAH average value in temperature range 295–403 K

Name: *N*–(2–Aminoethyl)–*N*'–[2–[(2–aminoethyl)amino]ethyl]–1,2–ethanediamine
Formula: $C_8H_{23}N_5$

CAS–RN: 112–57–2
Group No.: 31–036
Molar Mass: 189.30

TABLE 31.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	333.1–513.2	10	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 31.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.104	3.77–1	0.62	3.26–3	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
333.1–513.2		2.17416+1	1.34012+1	–9.95201–1			VI

TABLE 31.36.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	2.42	2.45	2.48	2.51	2.53	2.56	2.59
C_{sat} (J K^{-1}mol^{-1})	458	464	469	475	480	485	489
Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	2.61	2.63	2.66	2.68	2.70	2.72	2.74
C_{sat} (J K^{-1}mol^{-1})	494	499	503	507	511	515	518
Temp. (K)	470	480	490	500	510		
c_{sat} (J K^{-1}g^{-1})	2.76	2.77	2.79	2.81	2.82		
C_{sat} (J K^{-1}mol^{-1})	522	525	528	531	534		

Name: Benzenepropanamine
Formula: $C_9H_{13}N$

CAS–RN: 2038–57–5
Group No.: 31–037
Molar Mass: 135.21

TABLE 31.37.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75NIC/WAD	298.15	1.964	nosp	99.5	chrom	C_p	BSIO	70LKB/COM

Name: *N,N*,2–Trimethylbenzenamine
Formula: $C_9H_{13}N$

CAS–RN: 609–72–3
Group No.: 31–038
Molar Mass: 135.21

TABLE 31.38.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
02LOU2	N	376.13	2.071	nosp	not specified		C_{avg}	DSIO	*98LOU

02LOU2 average value in temperature range 295–458 K

Name: 2–Naphthalenamine
Formula: $C_{10}H_9N$

CAS–RN: 91–59–8
Group No.: 31–039
Molar Mass: 143.19

TABLE 31.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
35SKA	N	386.0–396.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

35SKA temperature range not specified, recommended use near n.m.t.

TABLE 31.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	3.82–6	0.00	–7.63–7	0

Temp. range K	A_1	A_2	Level of uncertainty
386.0–396.0	–1.44938+1	1.29829+1	VI

TABLE 31.39.4. Recommended values of heat capacities

Temp. (K)	390	400
c_p ($J\,K^{-1}g^{-1}$)	2.10	2.17
C_p ($J\,K^{-1}mol^{-1}$)	300	311

Name: *N,N*–Diethylbenzenamine
Formula: $C_{10}H_{15}N$

CAS–RN: 91–66–7
Group No.: 31–040
Molar Mass: 149.24

TABLE 31.40.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH		318.2–347.6	6S	nosp	not specified		C_p	DSIO	*86SCH
34KOL/UDO2	N	302.3	1	nosp	not specified		C_p	BSIT	34KOL/UDO2

34KOL/UDO2 same datum in 34KOL/UDO1

TABLE 31.40.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*87SCH	318.2–347.6	6	3.00#	0.025	2.80–2	0.08	4.07–5	2

TABLE 31.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.031	3.43–2	0.09	4.07–5	2
Temp. range K		A_1	A_2				Level of uncertainty
318.2–347.6		1.42456+1	6.75821				V

TABLE 31.40.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	2.00	2.04	2.07	2.11
C_p ($J K^{-1} mol^{-1}$)	298	304	309	315

Name: (1,1'–Biphenyl)–2–amine
Formula: $C_{12}H_{11}N$

CAS–RN: 90–41–5
Group No.: 31–041
Molar Mass: 169.23

TABLE 31.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91STE/CHI	295.4–440.5	19	0.10	99.976	melpt	C_{sat}	BSAO	47HUF
91STE/CHI	320.0–800.0	25	1.00	99.976	melpt	C_{sat}	BDHT	89KNI/ARC

TABLE 31.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
91STE/CHI	295.4–440.5	19	0.10	0.389	1.55–2	0.04	–9.26–5	–2
91STE/CHI	320.0–800.0	25	1.00	0.242	1.40–1	0.24	8.81–3	2

TABLE 31.41.3. Parameters of cubic spline polynomials

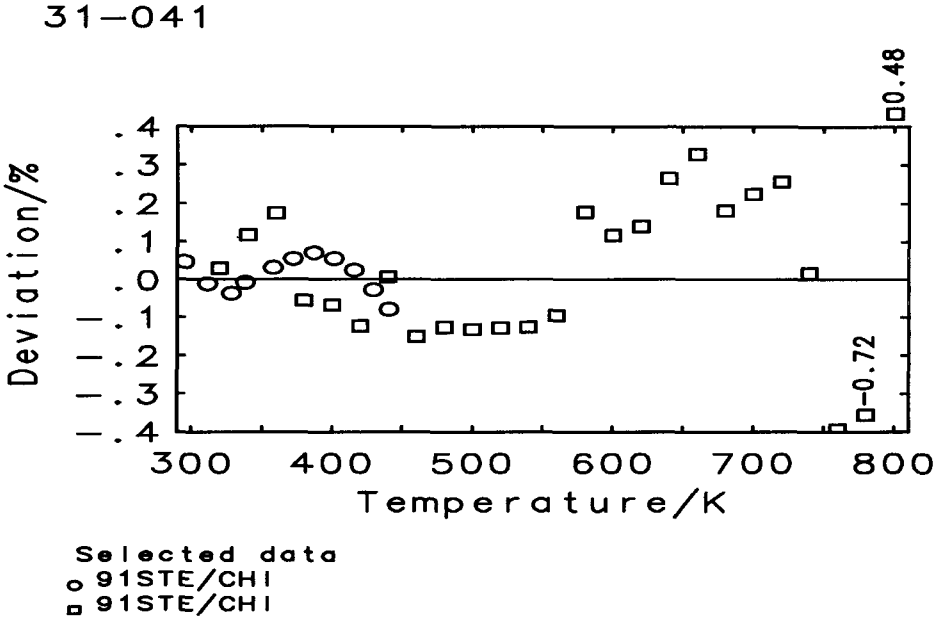
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	44	44	0.338	1.14–1	0.20	4.96–3	0
C_{sat}	44	44	0.328	9.47–2	0.17	4.65–3	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
295.4–450.0		2.05924+1	5.96035	–4.54151–1	5.71874–2		II
450.0–700.0		4.10479+1	–7.67666	2.57629	–1.67290–1		IV
700.0–800.0		–1.64282+3	7.13983+2	–1.00518+2	4.74196		IV
295.4–450.0		2.04101+1	6.11443	–4.97192–1	6.11582–2		II
450.0–700.0		4.39914+1	–9.60644	2.99634	–1.97622–1		IV
700.0–800.0		–7.67304+2	3.38092+2	–4.66748+1	2.16767		IV

TABLE 31.41.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J\,K^{-1}g^{-1}$)	1.812	1.836	1.860	1.884	1.908	1.932	1.957
C_p ($J\,K^{-1}mol^{-1}$)	306.7	310.7	314.7	318.8	322.9	327.0	331.1
c_{sat} ($J\,K^{-1}g^{-1}$)	1.812	1.836	1.860	1.884	1.908	1.932	1.957
C_{sat} ($J\,K^{-1}mol^{-1}$)	306.7	310.7	314.7	318.8	322.9	327.0	331.1
Temp. (K)	390	400	410	420	430	440	450
c_p ($J\,K^{-1}g^{-1}$)	1.981	2.006	2.031	2.056	2.082	2.108	2.134
C_p ($J\,K^{-1}mol^{-1}$)	335.3	339.5	343.7	348.0	352.3	356.7	361.1
c_{sat} ($J\,K^{-1}g^{-1}$)	1.981	2.006	2.031	2.056	2.082	2.108	2.134
C_{sat} ($J\,K^{-1}mol^{-1}$)	335.3	339.5	343.7	348.0	352.3	356.7	361.1
Temp. (K)	460	470	480	490	500	510	520
c_p ($J\,K^{-1}g^{-1}$)	2.160	2.187	2.214	2.241	2.268	2.295	2.322
C_p ($J\,K^{-1}mol^{-1}$)	365.6	370.1	374.6	379.2	383.8	388.4	393.0
c_{sat} ($J\,K^{-1}g^{-1}$)	2.160	2.187	2.214	2.241	2.268	2.295	2.323
C_{sat} ($J\,K^{-1}mol^{-1}$)	365.6	370.1	374.7	379.2	383.8	388.4	393.0
Temp. (K)	530	540	550	560	570	580	590
c_p ($J\,K^{-1}g^{-1}$)	2.350	2.377	2.404	2.431	2.457	2.484	2.510
C_p ($J\,K^{-1}mol^{-1}$)	397.6	402.2	406.8	411.3	415.8	420.3	424.7
c_{sat} ($J\,K^{-1}g^{-1}$)	2.350	2.377	2.403	2.430	2.456	2.482	2.507
C_{sat} ($J\,K^{-1}mol^{-1}$)	397.6	402.2	406.7	411.2	415.6	420.0	424.3
Temp. (K)	600	610	620	630	640	650	660
c_p ($J\,K^{-1}g^{-1}$)	2.535	2.560	2.585	2.609	2.633	2.656	2.678
C_p ($J\,K^{-1}mol^{-1}$)	429.0	433.3	437.5	441.6	445.6	449.4	453.2
c_{sat} ($J\,K^{-1}g^{-1}$)	2.532	2.556	2.580	2.603	2.625	2.647	2.668
C_{sat} ($J\,K^{-1}mol^{-1}$)	428.5	432.6	436.6	440.5	444.3	447.9	451.4
Temp. (K)	670	680	690	700	710	720	730
c_p ($J\,K^{-1}g^{-1}$)	2.700	2.721	2.741	2.760	2.778	2.797	2.818
C_p ($J\,K^{-1}mol^{-1}$)	456.9	460.4	463.8	467.0	470.1	473.3	476.9
c_{sat} ($J\,K^{-1}g^{-1}$)	2.687	2.706	2.724	2.741	2.756	2.772	2.787
C_{sat} ($J\,K^{-1}mol^{-1}$)	454.8	458.0	461.0	463.8	466.5	469.0	471.6
Temp. (K)	740	750	760	770	780	790	800
c_p ($J\,K^{-1}g^{-1}$)	2.842	2.871	2.906	2.948	2.999	3.060	3.133
C_p ($J\,K^{-1}mol^{-1}$)	480.9	485.8	491.7	498.8	507.5	517.9	530.3
c_{sat} ($J\,K^{-1}g^{-1}$)	2.803	2.821	2.840	2.863	2.888	2.918	2.952
C_{sat} ($J\,K^{-1}mol^{-1}$)	474.4	477.3	480.7	484.4	488.8	493.8	499.6

TABLE 31.41.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	44	44	0.840	4.12–1	0.74	7.51–2	7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
295.4–800.0	838.00	–1.34844	1.16765–2	2.13538+1	3.89306+1		IV



Name: *N*–Phenylbenzenamine
Formula: $C_{12}H_{11}N$

CAS–RN: 122–39–4
Group No.: 31–042
Molar Mass: 169.23

TABLE 31.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*84BAT	N	326.1–339.1	2	nosp	not specified	C_p	not specified	
13CAM	N	327.1–329.1	2	nosp	not specified	C_p	not specified	

*84BAT error 0.5 % (information in 29WAS)
13CAM error 0.5 % (information in 29WAS)

TABLE 31.42.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
*84BAT	326.1–339.1	2	5.00#	0.581	1.15	2.90	9.58–1	2
13CAM	327.1–329.1	2	5.00#	0.455	8.54–1	2.28	–8.52–1	–2

TABLE 31.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.738	1.43	3.69	5.27–2	0
Temp. range K		A_1	A_2				Level of uncertainty
326.1–339.1		–3.22463+1	2.15174+1				VI

TABLE 31.42.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p ($J\,K^{-1}g^{-1}$)	1.90	2.01
C_p ($J\,K^{-1}mol^{-1}$)	322	340

Name: *N*–Methyl–*N*–phenylbenzenamine
Formula: $C_{13}H_{13}N$

CAS–RN: 552–82–9
Group No.: 31–043
Molar Mass: 183.25

TABLE 31.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	322.7–375.2	3S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 31.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.234	2.94–1	0.70	1.44–3	1
Temp. range K		A_1	A_2				Level of uncertainty
322.7–375.2		1.47299+1	7.28325				V

TABLE 31.43.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J\,K^{-1}g^{-1}$)	1.73	1.76	1.79	1.82	1.86	1.89	1.92
C ($J\,K^{-1}mol^{-1}$)	316	322	328	334	340	347	353

Name: 4,4'–Methylenebisbenzenamine
Formula: $C_{13}H_{14}N_2$

CAS–RN: 101–77–9
Group No.: 31–044
Molar Mass: 198.27

TABLE 31.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
66ZAL/STR	N	388.1	1	nosp	not specified	C_{avg}	not specified	
78MAR/CIO1	N	370.0–470.0	11S	nosp	not specified	C_p	DSIO	71MAR/CIO
87LES/LIC	N	350.0–410.0	eqn	2.00	99. estim	C_p	BDHT	69PER/COM

66ZAL/STR average value in temperature range 383–393 K
78MAR/CIO1 values calculated from temperature dependence of enthalpy by the authors
87LES/LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 31.44.2. Correlated heat capacities

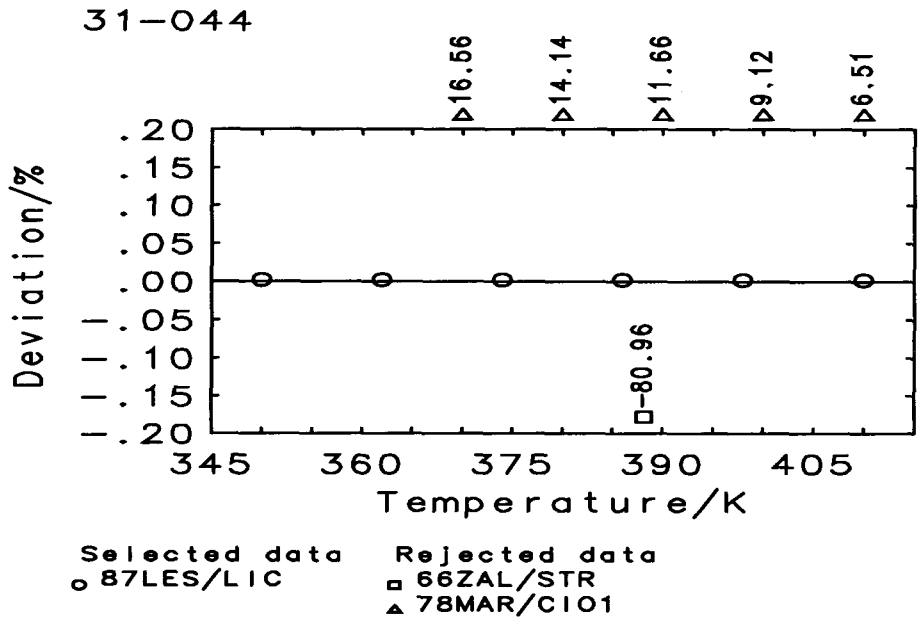
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
87LES/LIC	350.0–410.0	6	2.00	0.000	3.12–6	0.00	0.00	0
				Rejected data				
66ZAL/STR	(2.21+1, 80.96, –2.21+1, –1)			78MAR/CIO1	(6.88, 12.13, 6.55, 5)			

TABLE 31.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	6	0.000	3.82–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
350.0–410.0		1.81840+1	8.06038				V

TABLE 31.44.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	1.95	1.98	2.01	2.05	2.08	2.11	2.15
C_p (J K^{-1}mol^{-1})	386	392	399	406	413	419	426



Name: *N,N*–Dimethyl–2–pentyl–1–nonanamine
Formula: $C_{16}H_{35}N$

CAS–RN: 99916–30–0
Group No.: 31–045
Molar Mass: 241.46

TABLE 31.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87MIL/FEN2	323.1–423.1	21	1.50	99.9	chrom	C_p	BDHT	87PER/COM

TABLE 31.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	20	0.206	2.18–1	0.31	1.18–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
323.1–423.1		2.66340+1	1.17152+1				V

TABLE 31.45.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.21	2.25	2.29	2.33	2.37	2.41	2.45
C_p (J K^{-1}mol^{-1})	533	543	553	562	572	582	592
Temp. (K)	390	400	410	420			
c_p (J K^{-1}g^{-1})	2.49	2.53	2.57	2.61			
C_p (J K^{-1}mol^{-1})	601	611	621	63			

TABLE 31.45.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	20	0.211	2.22–1	0.32	1.21–3	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
323.1–423.1	702.00	5.54263	8.19602–2	2.45906+1	9.37062+1		V

32. Nitriles

The family of nitriles contains 26 compounds 11 of which were measured at a single temperature, with two compounds at two temperatures.

The largest number of measurements was performed at UMAA where four aliphatic dinitriles (63WUL/WES, 65CLE/WUL, 67RIB/WES, 68GIR/WES) and one mononitrile (67WES/RIB) were studied. These results are believed to be among the most reliable in this family. The measurements for propanenitrile and acetonitrile from RUH (62WEB/KIL, 65PUT/MCE), for acrylonitrile from BMB (72FIN/MES), and for cyanogen from UCB (39RUE/GIA) are also considered to be of good quality. All have been included in the final correlation.

The measurements for five nitriles were performed at APIB (85GUS/MIR, 87MIR/SHA) with a claimed error of 1.9 %, however, results for three of the five measured compounds obtained from other laboratories were available and showed differences of 5 to 20 % compared to the data from APIB. Therefore, only the data for the two remaining compounds, 2-methyl-2-propanenitrile and butanenitrile, have been included as no other information was available.

Two sets of data were reported for 1,2-benzenecarbonitrile covering almost the same temperature range. The work was performed in cooperation between the Institute of Elementary Organic Compounds, Academy of Science, Moscow and GPI (82KAR/SHV, 84RAB/KAR). The values in the two sets differed by 2 to 3 % with no explanation for the difference, and as a result, both were used in the final correlation.

The largest amount of data appears for acetonitrile which is often used in excess heat capacity studies. Recommended values are based upon experimental data from RUH (65PUT/MCE) and those supplemented by calculated values derived from an equation published by (71GOP/GAM) from IISB.

Recommended data for benzonitrile which was also frequently measured are based on reliable data from GPI (83BYK/LEB2) and were supplemented by three values derived from the excess heat capacity measurements at OCUO (85TAN/NAK).

Name: Ethanedinitrile
Formula: C_2N_2

CAS-RN: 460-19-5
Group No.: 32-001
Molar Mass: 52.04

TABLE 32.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
39RUE/GIA	246.3–253.8	4	0.20	99.995	melpt	C_p	BSIO	37GIA/EGA

TABLE 32.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.148	3.74–3	0.03	3.17–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
246.3–253.8		3.75239+2	−2.91329+2	5.85131+1			II

TABLE 32.1.4. Recommended values of heat capacities

Temp. (K)	246	248	250	252	254
c_p ($J K^{-1} g^{-1}$)	2.024	2.017	2.017	2.025	2.040
C_p ($J K^{-1} mol^{-1}$)	105.3	104.9	105.0	105.4	106.1

TABLE 32.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
00LOU	N	321.7	1	nosp	not specified	C_{avg}	DSIO	*98LOU
07WAL		291.1	1	nosp	not specified	C_{avg}	DSIO	07WAL
65PUT/MCE		234.2–300.6	9	0.30	99.72 melpt	C_p	BSIO	55TAY/JOH
71GOP/GAM		318.0–333.0	eqn	1.00	not specified	C_p	BSAO	71GOP/GAM
71HAL/BAL	N	297.1	1	nosp	99.9 chrom	C_p	BDHT	71DU/COM
78DEV/HEU		298.1	1	1.00	99.8 chrom	C_p	BSIO	70LKB/COM
79DEV/SOM		298.1	1	1.00	99.8 chrom	C_p	BSIO	70LKB/COM
84GUS/MIR		303.1–343.1	3S	1.60	not specified	C_p	BDHT	84GUS/MIR
87MIR/SHA		253.0–353.0	6	1.90	not specified	C_p	BDHT	84GUS/MIR
91GRO/ROU		298.1	1	nosp	99.5 anal	C_p	FSIT	71PIC/LED
91KAL/KOH		293.1–313.1	2	1.00	99.95 anal	C_p	FSIT	71PIC/LED
92PIE/SOM		278.1	1	nosp	99.5 chrom	C_p	FSIT	71PIC/LED

00LOU average value in temperature range 294–350 K
71HAL/BAL suspect value

TABLE 32.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65PUT/MCE	234.2–300.6	9	0.30	0.076	2.44–3	0.02	–7.61–4	–4
71GOP/GAM	318.0–333.0	6	1.00	0.010	1.10–3	0.01	–1.01–3	–3
78DEV/HEU	298.1	1	1.00	0.267	2.95–2	0.27	2.95–2	1
79DEV/SOM	298.1	1	1.00	0.267	2.95–2	0.27	2.95–2	1
92PIE/SOM	278.1	1	0.50#	0.110	5.95–3	0.05	5.95–3	1
				Rejected data				
00LOU	(4.95–2, 0.44,–4.95–2, –1)			07WAL	(2.35–1, 2.19,–2.35–1, –1)			
71HAL/BAL	(1.07, 10.74, –1.07, –1)			84GUS/MIR	(1.56, 16.30, –1.55, –2)			
87MIR/SHA	(1.71, 18.74, –1.70, –5)			91GRO/ROU	(1.87–1, 1.73,–1.87–1, –1)			
91KAL/KOH	(6.19–1, 6.00,–6.01–1, –2)							

TABLE 32.2.3. Parameters of regression polynomial

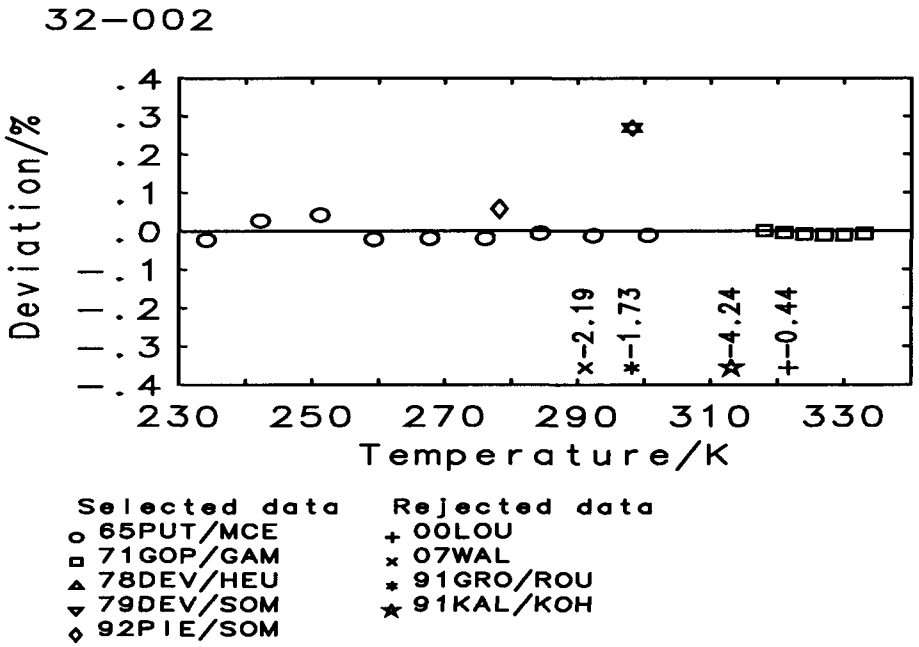
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	18	0.122	1.15–2	0.10	2.89–3	–4
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
234.2–333.0	1.69949+1	–7.42012	2.64468	–2.78522–1			III

TABLE 32.2.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	2.133	2.141	2.151	2.164	2.179	2.184	2.195
C_p ($J\,K^{-1}mol^{-1}$)	87.55	87.88	88.32	88.84	89.45	89.65	90.12
Temp. (K)	290	298.15	300	310	320	330	
c_p ($J\,K^{-1}g^{-1}$)	2.213	2.228	2.231	2.250	2.269	2.289	
C_p ($J\,K^{-1}mol^{-1}$)	90.84	91.45	91.60	92.38	93.17	93.95	

TABLE 32.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	18	0.234	1.69–2	0.15	5.09–3	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
234.2–333.0	545.50	–3.37672–1	8.22775–1	8.88727	3.46457–2		III



Name: Propanedinitrile
Formula: $C_3H_2N_2$

CAS–RN: 109–77–3
Group No.: 32–003
Molar Mass: 66.06

TABLE 32.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
68GIR/WES	310.6–319.2	5	0.20	99.9	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 32.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	5	1.375	4.31–2	0.28	1.43–4	1
Temp. range K		A_1	A_2				Level of uncertainty
310.6–319.2		1.36678	4.59229				II

TABLE 32.3.4. Recommended values of heat capacities

Temp. (K)	310	320
c_{sat} (J K^{-1}g^{-1})	1.964	2.022
C_{sat} (J K^{-1}mol^{-1})	129.7	133.5

Name: 2-Propenenitrile
Formula: C_3H_3N

CAS-RN: 107-13-1
Group No.: 32-004
Molar Mass: 53.06

TABLE 32.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
45DAV/WIE		294.6–312.9	4	nosp	99.	anal	C_{avg}	DSIO	45DAV/WIE
67LEB/RAB3		190.1–300.0	13S	0.50	not specified		C_p	BSAO	56POP/KOL
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM
72FIN/MES		196.7–347.1	18	0.20	99.92	melpt	C_{sat}	BSAO	47HUF
87MIR/SHA		213.0–333.0	7	1.90	not specified		C_p	BDHT	84GUS/MIR

71HAL/BAL suspect value

TABLE 32.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
72FIN/MES	196.7–347.1	18	0.20	0.126	3.26–3	0.03	2.33–6	–2
				Rejected data				
45DAV/WIE	(5.18–1, 3.83, 2.49–1, 2)			67LEB/RAB3	(2.94–1, 2.35, –2.33–1, –10)			
71HAL/BAL	(2.44–1, 1.90,–2.44–1, –1)			87MIR/SHA	(1.36, 12.12, –1.33, –7)			

TABLE 32.4.3. Parameters of regression polynomial

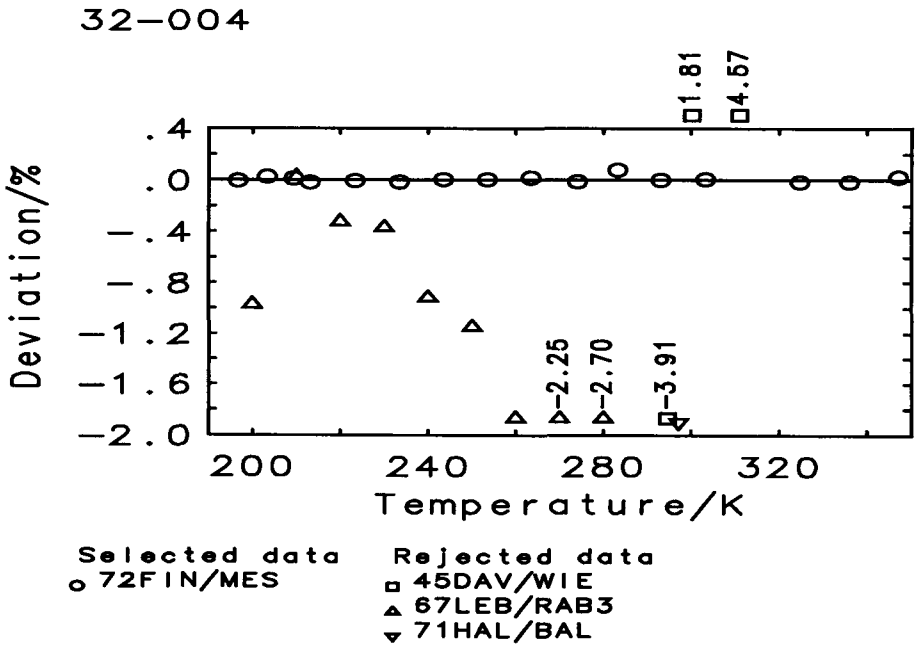
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	43	18	0.143	3.69–3	0.03	2.33–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
196.7–347.1		1.58738+1	–4.35640	1.56203	–1.39086–1		II

TABLE 32.4.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} ($J\,K^{-1}g^{-1}$)	1.927	1.931	1.938	1.947	1.958	1.970	1.984
C_{sat} ($J\,K^{-1}mol^{-1}$)	102.2	102.5	102.8	103.3	103.9	104.5	105.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} ($J\,K^{-1}g^{-1}$)	2.000	2.005	2.016	2.035	2.050	2.054	2.074
C_{sat} ($J\,K^{-1}mol^{-1}$)	106.1	106.4	107.0	108.0	108.8	109.0	110.1
Temp. (K)	320	330	340	350			
c_{sat} ($J\,K^{-1}g^{-1}$)	2.095	2.117	2.139	2.162			
C_{sat} ($J\,K^{-1}mol^{-1}$)	111.2	112.3	113.5	114.7			

TABLE 32.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	43	18	0.925	2.36–2	0.19	7.02–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
196.7–347.1	536.00	4.89427–1	1.44147	1.01848+1	4.15441–2		II



Name: Propanenitrile
Formula: C_3H_5N

CAS–RN: 107–12–0
Group No.: 32–005
Molar Mass: 55.08

TABLE 32.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81BER/OGI		243.1–363.1	5S	nosp	not specified	C_{avg}	DSIO	*79BER
00LOU	N	330.3	1	nosp	not specified	C_{avg}	DSIO	*98LOU
07WAL		290.1	1	nosp	not specified	C_p	DSIO	07WAL
62WEB/KIL		185.4–297.0	24	0.30	99.958 melpt	C_p	BSIO	55TAY/JOH
71HAL/BAL	N	297.1	1	nosp	99.9 chrom	C_p	BDHT	71DU/COM
85GUS/MIR		303.1–363.1	4	1.70	not specified	C_p	BDHT	84GUS/MIR
87MIR/SHA		193.0–353.0	9	1.90	not specified	C_p	BDHT	84GUS/MIR

00LOU average value in temperature range 292–368 K
71HAL/BAL suspect value

TABLE 32.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
00LOU	330.3	1	3.00#	0.135	6.04–2	0.41	–6.04–2	–1
62WEB/KIL	185.4–297.0	24	0.30	0.429	1.72–2	0.13	7.01–5	–3
				Rejected data				
*81BER/OGI	(1.40, 10.19, 4.72–2, 1)			07WAL	(4.28–2, 0.30, 4.28–2, 1)			
71HAL/BAL	(7.89–1, 5.81,–7.89–1, –1)			85GUS/MIR	(1.67, 12.89, –1.67, –2)			
87MIR/SHA	(1.78, 14.85, –1.78, –7)							

TABLE 32.5.3. Parameters of regression polynomial

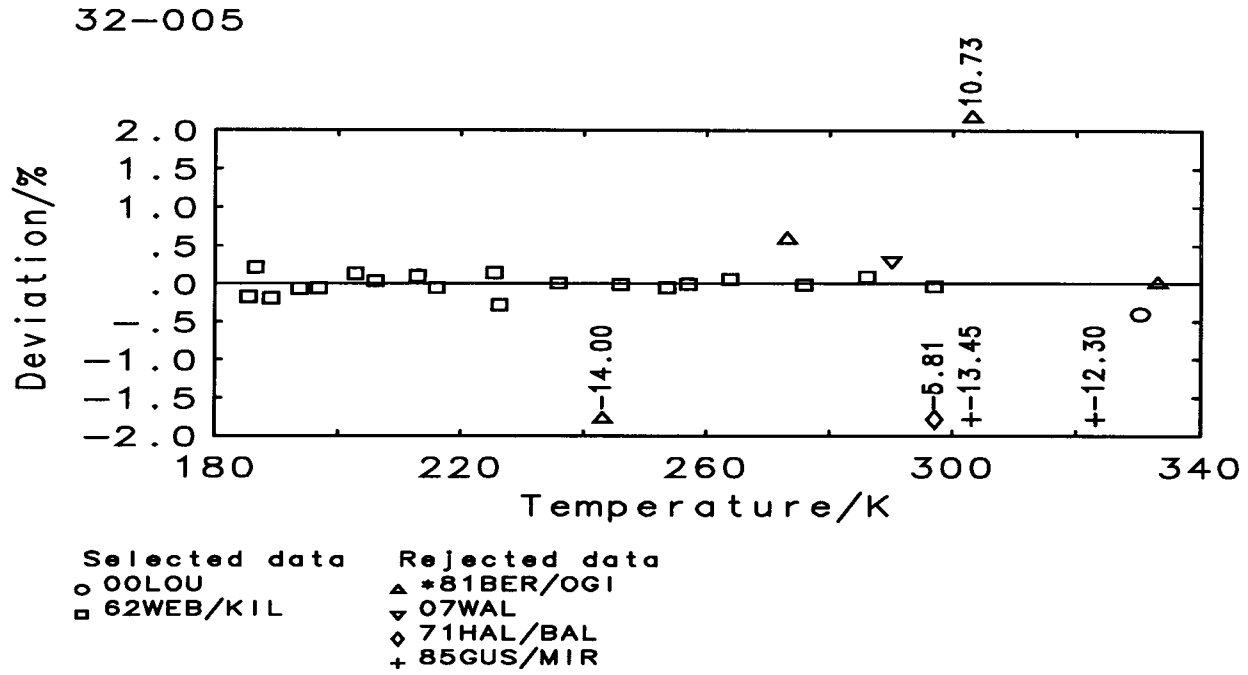
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	25	0.449	2.22–2	0.16	–2.35–3	–4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
185.4–330.3		1.46337+1	–1.79023	5.72505–1			II

TABLE 32.5.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	2.008	2.014	2.023	2.033	2.045	2.058	2.074
C_p (J K^{-1}mol^{-1})	110.6	110.9	111.4	112.0	112.6	113.4	114.2
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.091	2.109	2.116	2.130	2.152	2.172	2.176
C_p (J K^{-1}mol^{-1})	115.2	116.2	116.5	117.3	118.5	119.6	119.9
Temp. (K)	310	320	330				
c_p (J K^{-1}g^{-1})	2.202	2.229	2.258				
C_p (J K^{-1}mol^{-1})	121.3	122.8	124.4				

TABLE 32.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	25	0.622	2.64–2	0.19	2.21–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
185.4–330.3	561.30	3.55565	3.38952	9.31207	9.32482–1		II



Name: Butanedinitrile
Formula: $C_4H_4N_2$

CAS–RN: 110–61–2
Group No.: 32–006
Molar Mass: 80.09

TABLE 32.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63WUL/WES	334.0–347.6	8	0.80	99.93	melpt	C_p	BSAO	68WES/FUR

TABLE 32.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.089	1.38–2	0.07	1.43–5	1
Temp. range K		A_1	A_2				Level of uncertainty
334.0–347.6		1.39887+1	1.58442				IV

TABLE 32.6.4. Recommended values of heat capacities

Temp. (K)	335	340	345	350
c_p ($J K^{-1} g^{-1}$)	2.003	2.012	2.020	2.028
C_p ($J K^{-1} mol^{-1}$)	160.4	161.1	161.8	162.4

Name: Cyclopropanecarbonitrile
Formula: C_4H_5N

CAS-RN: 5500-21-0
Group No.: 32-007
Molar Mass: 67.09

TABLE 32.7.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71HAL/BAL	N	297.15	1.720	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: 2-Methyl-2-propenenitrile
Formula: C_4H_5N

CAS-RN: 126-98-7
Group No.: 32-008
Molar Mass: 67.09

TABLE 32.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
87MIR/SHA	253.0-353.0	6	1.90	not specified		C_p	BDHT	84GUS/MIR

TABLE 32.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.130	3.71-2	0.25	6.83-5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
253.0-353.0		1.99318+1	-5.92957	1.45349			VI

TABLE 32.8.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	1.76	1.78	1.80	1.81	1.82	1.85	1.88
C_p ($J K^{-1} mol^{-1}$)	118	119	121	121	122	124	126
Temp. (K)	300	310	320	330	340	350	
c_p ($J K^{-1} g^{-1}$)	1.89	1.92	1.96	2.01	2.05	2.10	
C_p ($J K^{-1} mol^{-1}$)	127	129	132	135	138	141	

TABLE 32.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.203	5.80–2	0.39	2.09–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
253.0–353.0	556.00	3.93049	4.79741	7.43006	8.05058–1	VI

Name: Butanenitrile
Formula: C_4H_7N

CAS–RN: 109–74–0
Group No.: 32–009
Molar Mass: 69.11

TABLE 32.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
02LOU2	N	340.4	1	nosp	not specified		C_{avg}	DSIO	*98LOU
85GUS/MIR		303.1–383.1	5	1.70	not specified		C_p	BDHT	84GUS/MIR
87MIR/SHA		173.0–373.0	11	1.90	not specified		C_p	BDHT	84GUS/MIR

02LOU2 average value in temperature range 294–386 K

TABLE 32.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
85GUS/MIR	303.1–383.1	5	1.70	0.109	3.26–2	0.18	2.01–3	3
87MIR/SHA	173.0–373.0	11	1.90	0.150	4.35–2	0.29	–3.68–3	–1
				Rejected data				
02LOU2	(2.02, 10.61, 2.02, 1)							

TABLE 32.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	16	0.033	9.80–3	0.06	1.40–4	–2

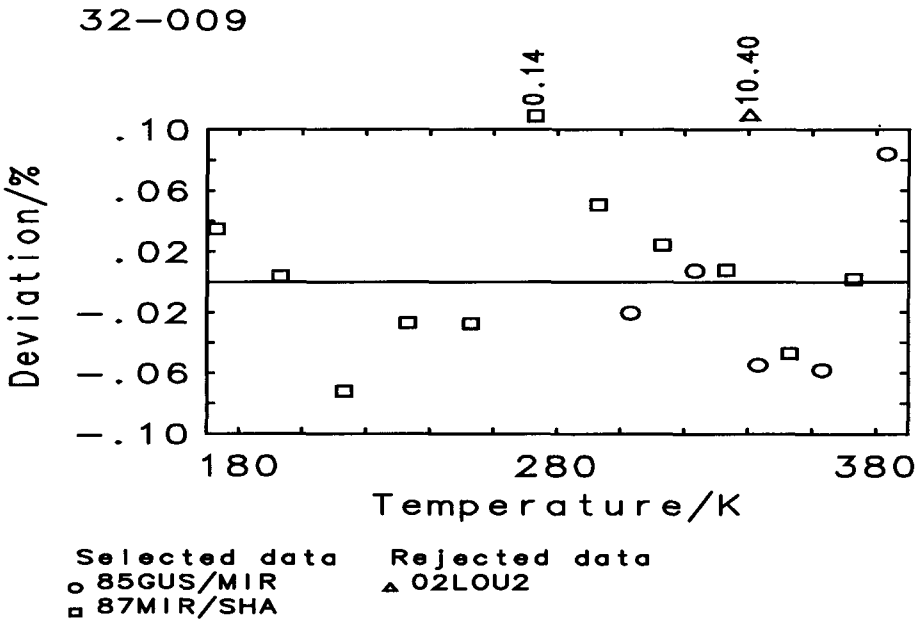
Temp. range K	A_1	A_2	A_3	Level of uncertainty
173.0–383.1	1.58008+1	–1.69392	6.05239–1	V

TABLE 32.9.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1} g^{-1}$)	1.77	1.77	1.78	1.78	1.79	1.81	1.82
C_p ($J K^{-1} mol^{-1}$)	122	122	123	123	124	125	126
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1} g^{-1}$)	1.83	1.85	1.86	1.88	1.89	1.90	1.92
C_p ($J K^{-1} mol^{-1}$)	127	128	129	130	130	131	133
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.94	1.95	1.97	1.99	2.02	2.05	2.08
C_p ($J K^{-1} mol^{-1}$)	134	134	136	138	140	142	144
Temp. (K)	360	370	380				
c_p ($J K^{-1} g^{-1}$)	2.11	2.14	2.18				
C_p ($J K^{-1} mol^{-1}$)	146	148	151				

TABLE 32.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	16	0.154	4.48–2	0.29	–1.90–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
173.0–383.1	585.40	1.23947–1	2.54412	1.10353+1	1.50964–3		V



Name: 2–Methylpropanenitrile
Formula: C_4H_7N

CAS–RN: 78–82–0
Group No.: 32–010
Molar Mass: 69.11

TABLE 32.10.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	2.260	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: Bicyclo[1.1.0]butane–1–carbonitrile
Formula: C_5H_5N

CAS–RN: 16955–35–4
Group No.: 32–011
Molar Mass: 79.10

TABLE 32.11.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	1.670	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: Dimethylpropanedinitrile
Formula: $C_5H_6N_2$

CAS–RN: 7321–55–3
Group No.: 32–012
Molar Mass: 94.12

TABLE 32.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67RIB/WES	309.0–346.1	7	0.10	99.93	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 32.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.830	1.91–2	0.08	2.21–5	0
Temp. range K		A_1	A_2				Level of uncertainty
309.0–346.1		1.60924+1	2.21299				II

TABLE 32.12.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c_{sat} (J $K^{-1}g^{-1}$)	2.028	2.047	2.067	2.086	2.106
C_{sat} (J $K^{-1}mol^{-1}$)	190.8	192.7	194.5	196.4	198.2

Name: Pentanedinitrile
Formula: $C_5H_6N_2$

CAS–RN: 544–13–8
Group No.: 32–013
Molar Mass: 94.12

TABLE 32.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65CLE/WUL	245.4–346.8	21	0.10	99.14	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 32.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.774	1.69–2	0.08	2.33–5	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
245.4–346.8		1.97967+1	–4.10976–1	3.91177–1			II

TABLE 32.13.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.874	1.888	1.903	1.908	1.918	1.934	1.948
C_{sat} (J K^{-1}mol^{-1})	176.4	177.7	179.1	179.5	180.5	182.0	183.3
Temp. (K)	300	310	320	330	340	350	
c_{sat} (J K^{-1}g^{-1})	1.951	1.968	1.987	2.005	2.025	2.045	
C_{sat} (J K^{-1}mol^{-1})	183.6	185.3	187.0	188.7	190.6	192.5	

TABLE 32.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.772	1.69–2	0.08	2.27–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
245.4–346.8	782.00	–1.26989–2	5.70198	1.28265+1	7.07041–6		II

Name: Cyclobutanecarbonitrile
Formula: C_5H_7N

CAS–RN: 4426–11–3
Group No.: 32–014
Molar Mass: 81.12

TABLE 32.14.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	1.800	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL *suspect value*

Name: 2,2–Dimethylpropanenitrile
Formula: C_5H_9N

CAS–RN: 630–18–2
Group No.: 32–015
Molar Mass: 83.13

TABLE 32.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67WES/RIB		295.6–345.6	7	0.10	99.98	melpt	C_{sat}	BSAO	68WES/FUR
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

TABLE 32.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67WES/RIB	295.6–345.6	7	0.10	0.840	1.88–2	0.08	3.54–5	1
				Rejected data				
71HAL/BAL	(3.15, 17.12, –3.15, –1)							

TABLE 32.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	7	0.994	2.23–2	0.10	3.54–5	1
Temp. range K		A_1	A_2				Level of uncertainty
295.6–345.6		1.41127+1	2.50181				II

TABLE 32.15.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_{sat} ($J K^{-1}g^{-1}$)	2.162	2.187	2.212	2.237	2.262	2.287
C_{sat} ($J K^{-1}mol^{-1}$)	179.7	181.8	183.9	186.0	188.1	190.1

Name: Pentanenitrile
Formula: C_5H_9N

CAS–RN: 110–59–8
Group No.: 32–016
Molar Mass: 83.13

TABLE 32.16.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
01KAH	N	345.15	2.175	nosp	not specified		C_{avg}	DSIO	01KAH

01KAH average value in temperature range 296–374 K

Name: Bicyclo[2.1.0]pentane–1–carbonitrile
Formula: C_6H_7N

CAS–RN: 31357–71–8
Group No.: 32–017
Molar Mass: 93.13

TABLE 32.17.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	1.760	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: 3–Methylenecyclobutanecarbonitrile
Formula: C_6H_7N

CAS–RN: 15760–35–7
Group No.: 32–018
Molar Mass: 93.13

TABLE 32.18.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	2.050	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: Cyclopentanecarbonitrile
Formula: C_6H_9N

CAS–RN: 4254–02–8
Group No.: 32–019
Molar Mass: 95.14

TABLE 32.19.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	1.760	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: Hexanenitrile
Formula: $C_6H_{11}N$

CAS–RN: 628–73–9
Group No.: 32–020
Molar Mass: 97.16

TABLE 32.20.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
00LOU	N	360.05	2.266	nosp	not specified		C_{avg}	DSIO	*98LOU

00LOU average value in temperature range 291–429 K

Name: Benzonitrile
Formula: C_7H_5N

CAS-RN: 100-47-0
Group No.: 32-021
Molar Mass: 103.12

TABLE 32.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
00LOU	N	376.6	1	nosp	not specified	C_{avg}	DSIO	*98LOU
83BYK/LEB2	N	265.3–328.9	14	0.30	99.88 melpt	C_p	BSAO	76LEB/LIT
85LAI/ROD		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
85TAN/NAK		283.1–318.1	3	0.30	99.9 chrom	C_p	FSIT	71PIC/LED
87MIR/SHA		273.0–453.0	10	1.90	not specified	C_p	BDHT	84GUS/MIR

00LOU average value in temperature range 294–459 K
83BYK/LEB2 smoothed values in 84LEB/BYK2

TABLE 32.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
00LOU	376.6	1	3.00#	0.700	4.81–1	2.10	4.81–1	1
83BYK/LEB2	265.3–328.9	14	0.30	1.275	7.69–2	0.38	–2.23–2	–6
85LAI/ROD	298.1	1	0.50#	0.647	6.46–2	0.32	6.46–2	1
85TAN/NAK	283.1–318.1	3	0.30	1.754	1.04–1	0.53	9.88–2	3
				Rejected data				
87MIR/SHA	(1.35, 6.90,–1.34, –6)							

TABLE 32.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	19	1.481	1.53–1	0.70	2.78–2	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
265.3–376.6	2.32023+1	–7.50760	2.95554	–2.70223–1			III

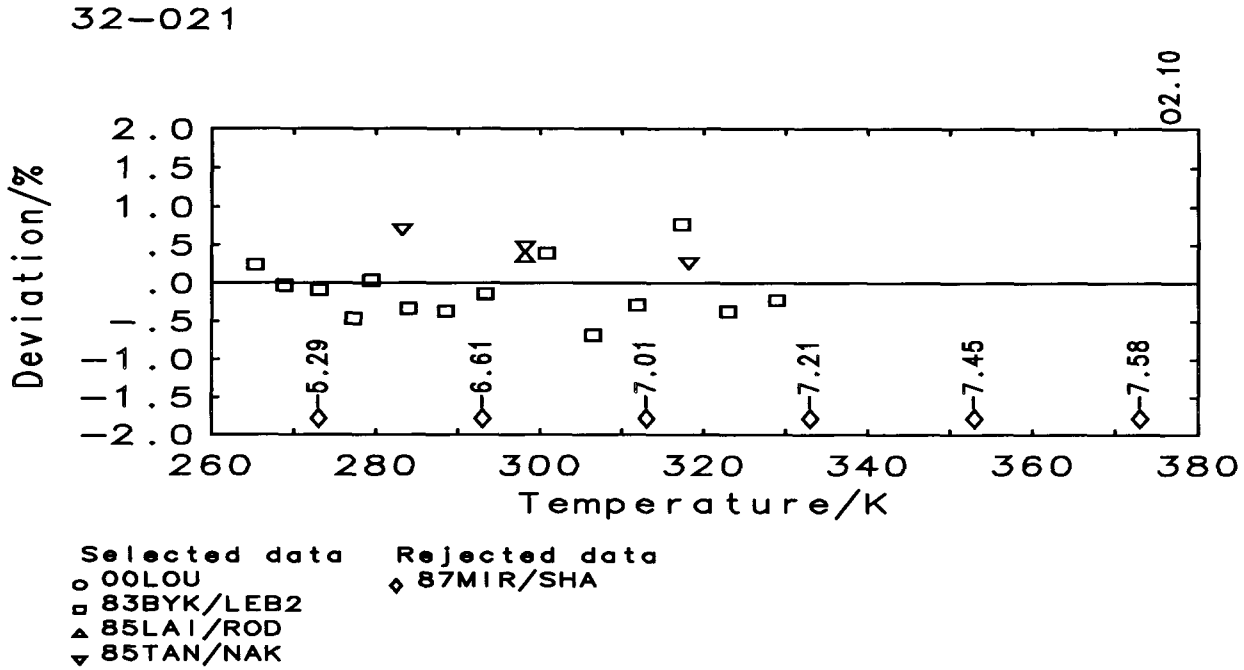
TABLE 32.21.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.545	1.551	1.566	1.588	1.607	1.611	1.635
C_p (J K^{-1}mol^{-1})	159.3	160.0	161.5	163.8	165.7	166.2	168.6
Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.660	1.685	1.711	1.737	1.763	1.790	1.816
C_p (J K^{-1}mol^{-1})	171.2	173.8	176.4	179.1	181.8	184.6	187.3

TABLE 32.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	19	1.456	8.91–2	0.44	4.60–3	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
265.3–376.6	699.40	5.57989	9.63365	5.88111	8.07978–1	III



Name: Bicyclo[3.1.0]hexane–1–carbonitrile
Formula: C_7H_9N

CAS–RN: 31357–72–9
Group No.: 32–022
Molar Mass: 107.16

TABLE 32.22.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71HAL/BAL	N	297.15	1.590	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: Cyclohexanecarbonitrile
Formula: $C_7H_{11}N$

CAS–RN: 766–05–2
Group No.: 32–023
Molar Mass: 109.17

TABLE 32.23.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71HAL/BAL	N	297.15	1.630	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: 1,2–Benzenedicarbonitrile
Formula: $C_8H_4N_2$

CAS–RN: 91–15–6
Group No.: 32–024
Molar Mass: 128.13

TABLE 32.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82KAR/SHV	420.8–480.4	15	1.50	99.66	melpt	C_p	BSAO	68LEA
84RAB/KAR	420.8–480.4	15	1.50	99.66	melpt	C_p	BSAO	76LEB/LIT

TABLE 32.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82KAR/SHV	420.8–480.4	15	1.50	1.104	4.49–1	1.66	4.32–1	15
84RAB/KAR	420.8–480.4	15	1.50	1.207	4.70–1	1.81	–4.00–1	–13

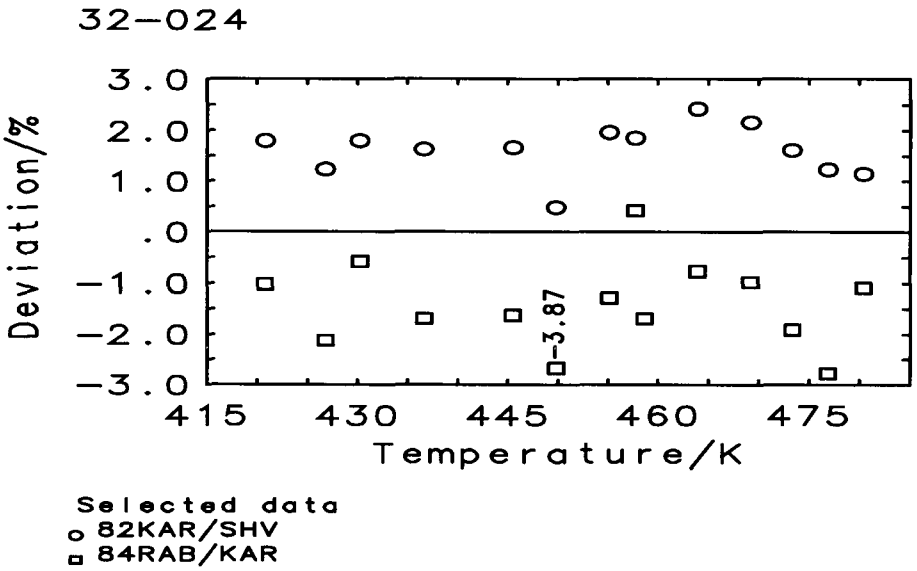
TABLE 32.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	30	30	1.219	4.85–1	1.83	1.60–2	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
420.8–480.4	1.60747+2	–6.26820+1	7.29067	V

TABLE 32.24.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	1.69	1.69	1.69	1.71	1.73	1.76	1.81
C_p (J K^{-1}mol^{-1})	217	216	217	219	222	226	232



Name: *endo*–Bicyclo[2.2.1]heptane–2–carbonitrile
Formula: $C_8H_{11}N$

CAS–RN: 3211–87–8
Group No.: 32–025
Molar Mass: 121.18

TABLE 32.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62SER/KOL	340.0–350.0	2S	nosp	99.88	melpt	C_p	BSAO	62KOL/SER

TABLE 32.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
340.0–350.0		9.21396	4.98183				IV

TABLE 32.25.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p (J K^{-1}g^{-1})	1.794	1.829
C_p (J K^{-1}mol^{-1})	217.4	221.6

Name: *exo*–Bicyclo[2.2.1]heptane–2–carbonitrile
Formula: $C_8H_{11}N$

CAS–RN: 3211–90–3
Group No.: 32–026
Molar Mass: 121.18

TABLE 32.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62SER/KOL	300.0–310.0	2S	nosp	99.82	melpt	C_p	BSAO	62KOL/SER

TABLE 32.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
300.0–310.0		7.92566	5.33410				IV

TABLE 32.26.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p (J K^{-1}g^{-1})	1.642	1.678
C_p (J K^{-1}mol^{-1})	198.9	203.4

33. Heterocyclic Nitrogen Compounds

This family contains 46 compounds of which five were measured at one temperature only.

The largest number of measurements for this family of compounds, which amounts to 26 substances, was performed at BMB (now called NIPER) where research was carried out on chemicals present in crude oil and fossil fuels. The measurements were made on 5- and 6-membered heterocyclic nitrogen compounds as well as compounds containing two and three condensed rings where one or two methylene (or CH groups) groups are replaced by nitrogen (57MCC/DOU, 59MCC/DOU, 63SCO/GOO, 63SCO/HUB, 67SCO/BER, 86STE/CHI, 88MES/TOD, 88STE/ARC, 89STE/CHI1, 89STE/CHI2, 92STE/CHI1). These measurements with a reported error between 0.1 and 0.2 % were the basis for recommended values in this family. In the case of the recent measurements for 9-methylcarbazole and 2,3,4,9-tetrahydro-9-methylcarbazole, two different instruments have been used; an adiabatic calorimeter at lower temperatures (measurement error of 0.1 %) and a DSC calorimeter at higher temperatures up to 700 K (measurement error of 1 %).

Measurements for compounds containing two or three nitrogen atoms in a ring were performed at SUU (79BRI/VAN, 83DEW/DEK, 83DEW/OFF) over a limited temperature range using adiabatic and DSC calorimetry (reported errors of 0.4 and 3 %, respectively). Two trimethylpyridines were measured with an estimated error of 0.4 % at ICTP (91SVO/ZAB1). Six derivatives of piperazine were studied by (88BOB/KAM) using samples having a low purity yielding results subjected to a high uncertainty (claimed error of 6 %). In both cases, all the data had to be used for the final recommendations as there were no other data available.

High precision measurements were performed on bridged nitrogen heterocycles at UMAA (63TRO/WES, 64WUL/WES). The only measurements on a 3-membered ring system containing nitrogen were performed at CIUG (77LEB/EVS2) for aziridine with a reported error of 0.3 %.

Two reliable data sets, one from BMB (59MCC/DOU) and the other from DCM (59HIL/SIN) were available for pyrrolidine showing excellent agreement. For all other compounds where several data sets were available the preference has been given to the results from BMB.

An unusual variation of the heat capacity for 3,4-dimethylpyridine was discussed by (84POD/RAC); the results obtained by collaboration of the three laboratories in Cracow and Gdansk (Poland) were presented only in the form of graphs and the direct experimental data were made available to us through the courtesy of the authors. A sharp lambda peak was observed near 293.5 K giving a 4 % increase in the heat capacity above the expected values. However, the data published for the same compound by (86STE/CHI) at BMB does not show any anomalous behavior. A discussion of these phenomena can be found in a paper by (93ZAB/BUR).

Name: Aziridine
Formula: C_2H_5N

CAS–RN: 151–56–4
Group No.: 33–001
Molar Mass: 43.07

TABLE 33.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
77LEB/EVS2	197.2–330.0	17S	0.30	not specified		C_p	BSAO	76LEB/LIT

TABLE 33.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.451	1.68–2	0.14	3.62–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
197.2–330.0		9.20516	4.80513–1	2.74965–1			III

TABLE 33.1.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	2.175	2.206	2.238	2.271	2.305	2.341	2.377
C_p ($J K^{-1}mol^{-1}$)	93.67	95.01	96.39	97.82	99.29	100.8	102.4
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	2.415	2.427	2.453	2.493	2.526	2.533	2.575
C_p ($J K^{-1}mol^{-1}$)	104.0	104.5	105.6	107.3	108.8	109.1	110.9
Temp. (K)	320	330					
c_p ($J K^{-1}g^{-1}$)	2.618	2.661					
C_p ($J K^{-1}mol^{-1}$)	112.7	114.6					

TABLE 33.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.487	1.77–2	0.15	4.33–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
197.2–330.0	547.00	–2.57588	4.30536–1	8.00215	3.85284		III

Name: 1,3,5–Triazine
Formula: $C_3H_3N_3$

CAS–RN: 290–87–9
Group No.: 33–002
Molar Mass: 81.08

TABLE 33.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79BRI/VAN	355.5–382.3	6	nosp	99.753	melpt	C_{sat}	BSAO	72VAN

TABLE 33.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	6	6	1.039	7.10–2	0.42	3.99–4	0
Temp. range K		A_1	A_2				Level of uncertainty
355.5–382.3		3.39125	3.73116				III

TABLE 33.2.4. Recommended values of heat capacities

Temp. (K)	360	370	380
c_{sat} ($J K^{-1}g^{-1}$)	1.725	1.764	1.802
C_{sat} ($J K^{-1}mol^{-1}$)	139.9	143.0	146.1

Name: 1*H*–Imidazole
Formula: $C_3H_4N_2$

CAS–RN: 288–32–4
Group No.: 33–003
Molar Mass: 68.08

TABLE 33.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DEW/DEK	367.2–375.0	3	nosp	99.78	melpt	C_p	BSAO	79SCH/OFF
83DEW/OFF	375.0–385.0	3S	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 33.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83DEW/DEK	367.2–375.0	3	0.40#	0.937	6.76–2	0.37	–1.03–2	–1
83DEW/OFF	375.0–385.0	3	3.00#	1.316	7.63–1	3.95	6.70–1	3

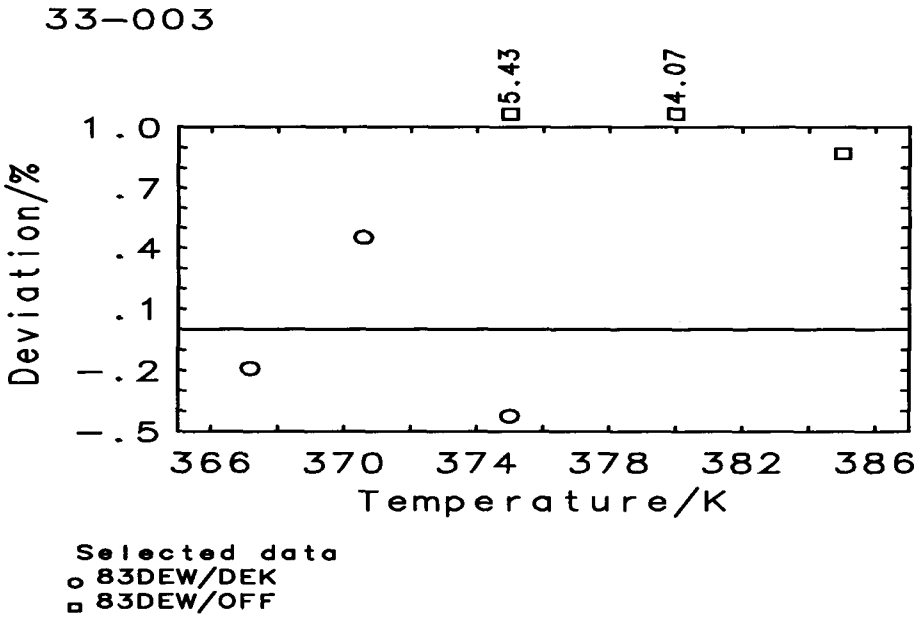
TABLE 33.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.616	7.66–1	3.97	3.30–1	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
367.2–385.0	1.21839+3	–6.48121+2	8.74814+1	V

TABLE 33.3.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_p ($J K^{-1} g^{-1}$)	2.19	2.29	2.60
C_p ($J K^{-1} mol^{-1}$)	149	156	177



Name: 1*H*-Pyrazole
Formula: $C_3H_4N_2$

CAS-RN: 288-13-1
Group No.: 33-004
Molar Mass: 68.08

TABLE 33.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83DEW/OFF	345.0–385.0	9S	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 33.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_t %	s_b/R	+/-
C_p	9	9	0.147	7.91–2	0.44	5.39–4	1
Temp. range K		A_1	A_2				Level of uncertainty
345.0–385.0		1.05269+1	2.09614				V

TABLE 33.4.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	2.18	2.21	2.23	2.26	2.28
C_p ($J K^{-1} mol^{-1}$)	149	150	152	154	155

Name: 1*H*–Pyrrole
Formula: C_4H_5N

CAS–RN: 109–97–7
Group No.: 33–005
Molar Mass: 67.09

TABLE 33.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67SCO/BER	256.1–359.7	20	0.20	99.994	melpt	C_{sat}	BSAO	47HUF

TABLE 33.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.225	6.74–3	0.05	1.16–5	–2

Temp. range K	A_1	A_2	Level of uncertainty
256.1–359.7	6.39423	3.00921	II

TABLE 33.5.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.762	1.799	1.811	1.837	1.874	1.904	1.911
C_{sat} (J K^{-1}mol^{-1})	118.2	120.7	121.5	123.2	125.7	127.8	128.2
Temp. (K)	310	320	330	340	350	360	
c_{sat} (J K^{-1}g^{-1})	1.949	1.986	2.023	2.060	2.098	2.135	
C_{sat} (J K^{-1}mol^{-1})	130.7	133.2	135.7	138.2	140.7	143.2	

TABLE 33.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.225	6.87–3	0.05	5.48–6	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
256.1–359.7	639.80	–3.81268–1	1.96258–3	6.49269	1.85170+1	II

Name: Pyrrolidine
Formula: C_4H_9N

CAS–RN: 123–75–1
Group No.: 33–006
Molar Mass: 71.12

TABLE 33.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59HIL/SIN	218.7–312.3	33	0.30	99.85	melpt	C_p	BSAO	58HIL/KRA
59MCC/DOU	218.4–350.6	22	0.20	99.85	melpt	C_{sat}	BSAO	47HUF
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA

TABLE 33.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59HIL/SIN	218.7–312.3	33	0.30	0.546	3.05–2	0.16	5.10–3	–1
59MCC/DOU	218.4–350.6	22	0.20	0.260	9.81–3	0.05	–3.33–3	–6
				Rejected data				
76CON/GIA	(4.49–1, 2.33, 4.49–1, 1)							

TABLE 33.6.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	56	55	0.476	2.56–2	0.14	1.73–3	–7
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
218.4–280.0	–4.77423+1	7.31612+1	–2.69820+1	3.33200			II
280.0–350.6	3.12749+1	–1.15000+1	3.25415	–2.67544–1			II

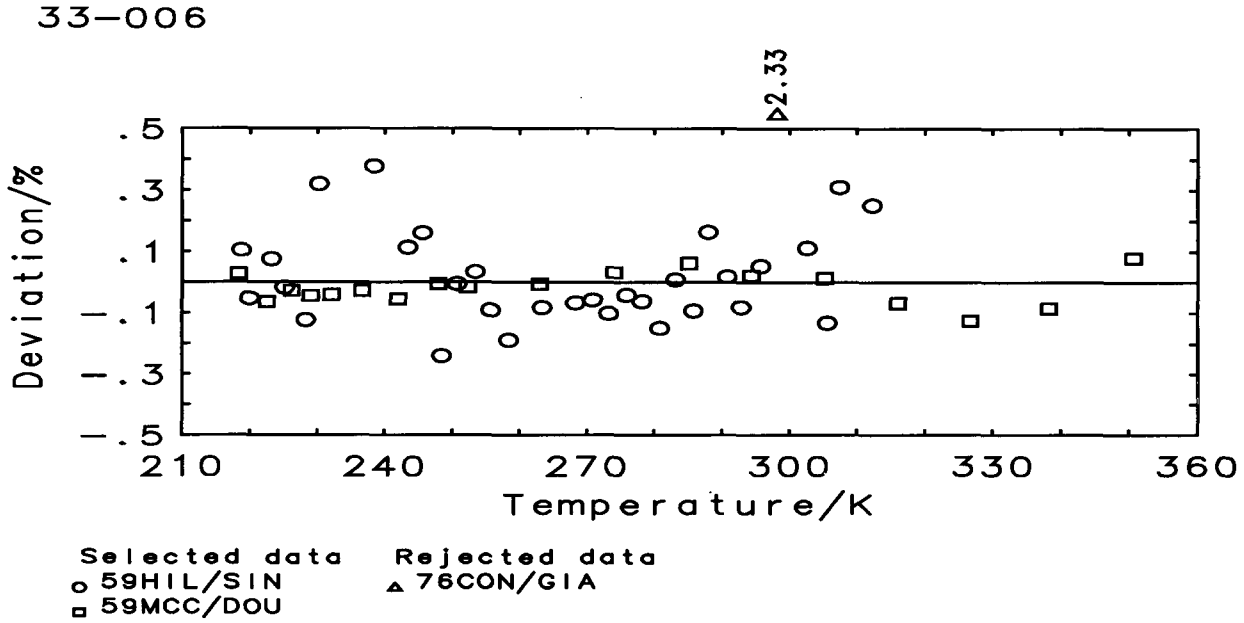
TABLE 33.6.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c ($J K^{-1} g^{-1}$)	2.116	2.143	2.162	2.173	2.179	2.184	2.185
C ($J K^{-1} mol^{-1}$)	150.5	152.4	153.7	154.5	155.0	155.3	155.4
Temp. (K)	280	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	2.188	2.194	2.201	2.202	2.213	2.225	2.238
C ($J K^{-1} mol^{-1}$)	155.6	156.0	156.5	156.6	157.4	158.2	159.2
Temp. (K)	340	350					
c ($J K^{-1} g^{-1}$)	2.254	2.270					
C ($J K^{-1} mol^{-1}$)	160.3	161.4					

TABLE 33.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	56	55	0.852	4.28–2	0.23	3.65–3	–8

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
218.4–350.6	568.60	2.58228+3	3.26889+2	–3.65675+2	2.67712+3	–1.81432+2	1.81885+3	II



Name: Piperazine
Formula: $C_4H_{10}N_2$

CAS–RN: 110–85–0
Group No.: 33–007
Molar Mass: 86.14

TABLE 33.7.1. *Experimental heat capacities*

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	413.1–473.1	4	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 33.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	0.089	1.62–1	0.53	4.56–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
413.1–473.1		–1.07568+2	5.73770+1	–5.91775			VI

TABLE 33.7.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440	450	460	470
c_{sat} (J K^{-1}g^{-1})	2.72	2.80	2.87	2.93	2.97	3.01	3.03
C_{sat} (J K^{-1}mol^{-1})	234	241	247	252	256	259	261

Name: Pyridine
Formula: C_5H_5N

CAS-RN: 110-86-1
Group No.: 33-008
Molar Mass: 79.10

TABLE 33.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
00LOU	N	337.7	1	nosp	not specified	C_{avg}	DSIO	*98LOU
16BRA		283.1–323.1	2	nosp	not specified	C_{avg}	DSTO	16BRA
17MAT/KRA		294.1	1	nosp	not specified	C_p	BSIO	49WEI
31SWI/RYB2	N	290.1	1	nosp	not specified	C_p	BDHT	31SWI/RYB2
34RAD/JUL		289.1	1	nosp	not specified	C_p	BSIO	49WEI
36PAR/TOD1	N	230.0–300.0	8S	0.70	not specified	C_p	BSIO	25PAR
36PEA/BAK		233.1–298.1	8S	nosp	not specified	C_p	BSIO	36PEA/BAK
47PUS/FED		284.0–306.9	5	nosp	not specified	C_p	DSIO	47PUS/FED
57MCC/DOU		239.7–346.7	13	0.20	99.92 melpt	C_{sat}	BSAO	47HUF
58SWI/ZIE1	N	332.1–348.8	2	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
67RAS/GAN		293.1–353.1	4S	0.50	not specified	C_p	BSAO	67RAS/GAN
92LAI/ROD		298.1	1	nosp	99.8 anal	C_p	FSIT	71PIC/LED

00LOU average value in temperature range 295–381 K
31SWI/RYB2 same datum in 31SWI/RYB1
36PAR/TOD1 high sample purity
58SWI/ZIE1 average values in temperature ranges 295–369 K and 295–402 K

TABLE 33.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
57MCC/DOU	239.7–346.7	13	0.20	0.055	1.72–3	0.01	8.07–7	0
				Rejected data				
00LOU	(1.88–1, 1.10, 1.88–1, 1)			16BRA	(1.89–1, 1.16,–5.85–2, 0)			
17MAT/KRA	(3.11–1, 2.00,–3.11–1, –1)			31SWI/RYB2	(5.14–1, 3.16, 5.14–1, 1)			
34RAD/JUL	(1.71–1, 1.10,–1.71–1, –1)			36PAR/TOD1	(1.67–1, 1.05, 1.49–1, 7)			
36PEA/BAK	(3.45–1, 2.43,–9.62–2, 1)			47PUS/FED	(1.95–1, 1.22, –1.20–1, –3)			
58SWI/ZIE1	(8.36–1, 4.73, 8.36–1, 1)			67RAS/GAN	(1.69–1, 1.00, 1.50–1, 3)			
92LAI/ROD	(1.48–1, 0.94,–1.48–1, –1)							

TABLE 33.8.3. Parameters of regression polynomial

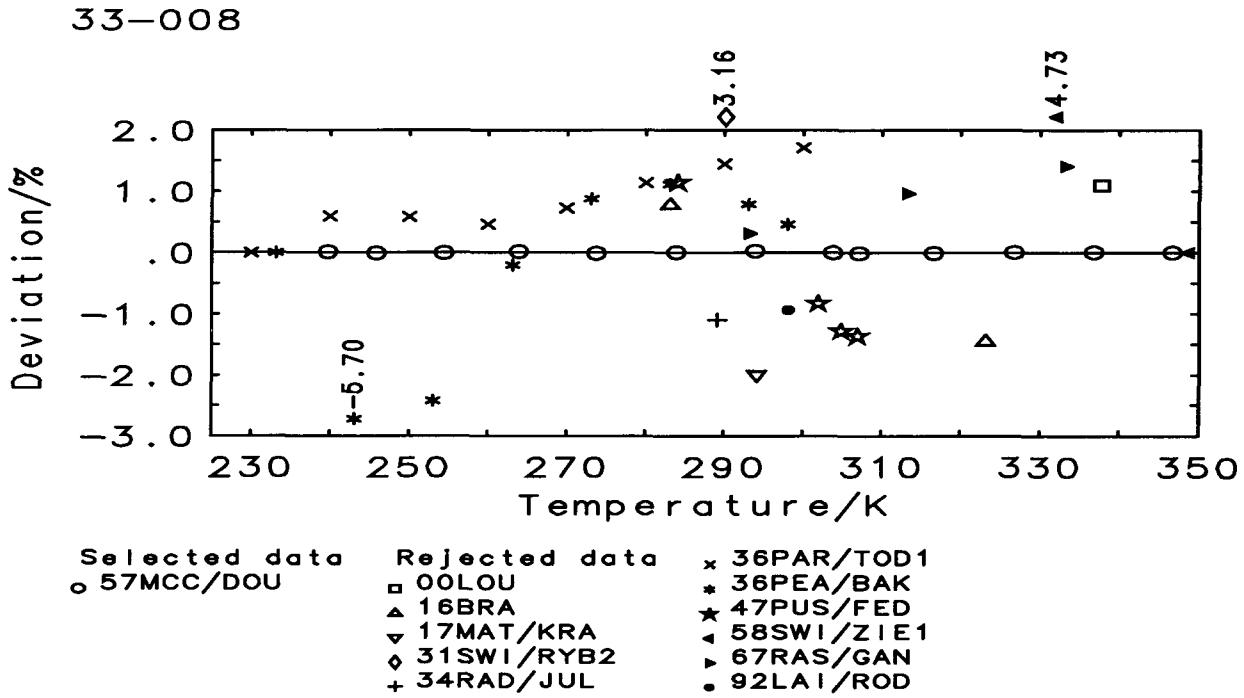
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	47	13	0.066	2.06–3	0.01	8.07–7	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
239.7–346.7		1.65422+1	–4.25000	1.83053	–1.57820–1		II

TABLE 33.8.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} ($J\,K^{-1}g^{-1}$)	1.546	1.565	1.586	1.609	1.616	1.632	1.657
C_{sat} ($J\,K^{-1}mol^{-1}$)	122.3	123.8	125.5	127.3	127.8	129.1	131.1
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} ($J\,K^{-1}g^{-1}$)	1.678	1.682	1.709	1.736	1.764	1.792	1.821
C_{sat} ($J\,K^{-1}mol^{-1}$)	132.7	133.1	135.2	137.3	139.5	141.8	144.0

TABLE 33.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	47	13	0.284	8.97–3	0.06	8.07–6	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
239.7–346.7	620.00	–3.70708	1.45022	9.59518	2.36904		II



Name: 1–Methyl–1*H*–pyrrole
Formula: C_5H_7N

CAS–RN: 96–54–8
Group No.: 33–009
Molar Mass: 81.12

TABLE 33.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
59MCC/DOU	N	230.0–340.0	12	nosp	not specified		C_{sat}	BSAO	47HUF
88MES/TOD	N	221.2–364.7	18	0.05	99.998	melpt	C_{sat}	BSAO	47HUF

59MCC/DOU data from a graph only
88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

TABLE 33.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59MCC/DOU	230.0–340.0	12	0.20#	0.569	1.95–2	0.11	–5.45–3	–3
88MES/TOD	221.2–364.6	18	0.05	0.522	4.81–3	0.03	2.31–4	3

TABLE 33.9.3. Parameters of regression polynomial

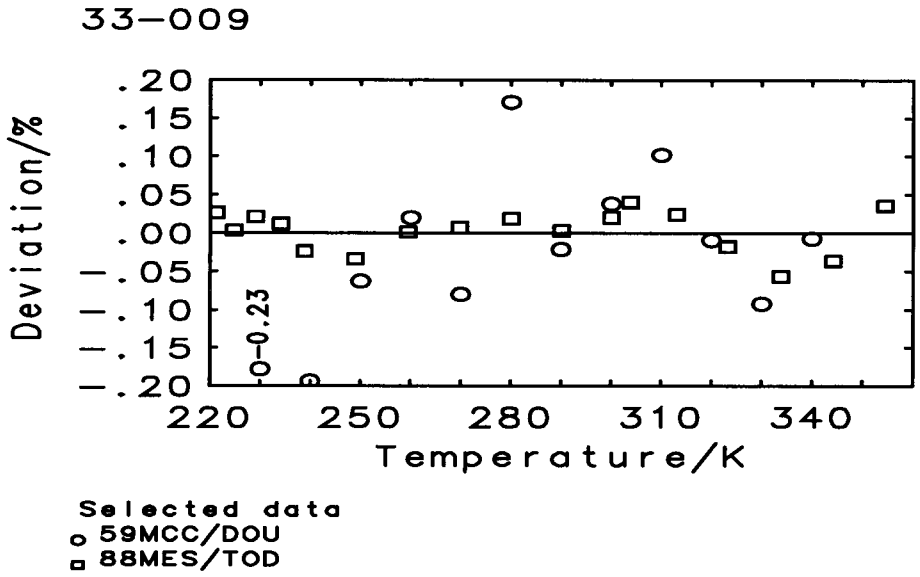
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.581	1.38–2	0.08	–2.04–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
221.2–364.6		2.22225+1	–8.10771	3.14301	–2.99713–1		II

TABLE 33.9.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J $K^{-1}g^{-1}$)	1.682	1.697	1.714	1.734	1.755	1.778	1.785
C_{sat} (J $K^{-1}mol^{-1}$)	136.4	137.6	139.1	140.6	142.4	144.2	144.8
Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J $K^{-1}g^{-1}$)	1.802	1.828	1.850	1.855	1.882	1.911	1.940
C_{sat} (J $K^{-1}mol^{-1}$)	146.2	148.3	150.0	150.4	152.7	155.0	157.3
Temp. (K)	340	350	360				
c_{sat} (J $K^{-1}g^{-1}$)	1.969	1.998	2.028				
C_{sat} (J $K^{-1}mol^{-1}$)	159.7	162.1	164.5				

TABLE 33.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	4.686	4.07–2	0.24	1.17–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
221.2–364.6	618.00	–4.05792	1.08190	1.14531+1	3.80504		II



Name: 1–Methylpyrrolidine
Formula: $C_5H_{11}N$

CAS–RN: 120–94–5
Group No.: 33–010
Molar Mass: 85.15

TABLE 33.10.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76CON/GIA	298.15	1.892	nosp	not specified		C_p	BDCT	76CON/GIA

Name: 3–Methylpyrrolidine
Formula: $C_5H_{11}N$

CAS–RN: 34375–89–8
Group No.: 33–011
Molar Mass: 85.15

TABLE 33.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86STE/CHI	170.4–400.0	26S	nosp	99.98	melpt	C_{sat}	BSAO	47HUF

TABLE 33.11.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	26	26	1.084	2.33–2	0.11	3.71–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
170.4–225.0		–2.04033+1	3.62398+1	–8.28510	2.59579–1		II
225.0–285.0		–7.16118+1	1.04518+2	–3.86309+1	4.75526		II
285.0–345.0		5.02929+1	–2.38028+1	6.39388	–5.10803–1		II
345.0–400.0		3.10498+1	–7.06977	1.54373	–4.21887–2		II

TABLE 33.11.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J $K^{-1}g^{-1}$)	1.810	1.904	1.985	2.052	2.106	2.147	2.175
C_{sat} (J $K^{-1}mol^{-1}$)	154.1	162.1	169.0	174.7	179.3	182.8	185.2
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J $K^{-1}g^{-1}$)	2.193	2.201	2.204	2.203	2.203	2.203	2.205
C_{sat} (J $K^{-1}mol^{-1}$)	186.7	187.4	187.6	187.6	187.6	187.6	187.7
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J $K^{-1}g^{-1}$)	2.209	2.210	2.220	2.232	2.247	2.265	2.286
C_{sat} (J $K^{-1}mol^{-1}$)	188.1	188.2	189.0	190.1	191.4	192.9	194.6
Temp. (K)	360	370	380	390	400		
c_{sat} (J $K^{-1}g^{-1}$)	2.308	2.333	2.359	2.388	2.419		
C_{sat} (J $K^{-1}mol^{-1}$)	196.5	198.6	200.9	203.3	206.0		

TABLE 33.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	26	26	9.462	2.18–1	0.95	3.12–3	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
170.4–400.0	577.00	1.97816+3	2.35449+2	–2.83467+2	2.23089+3	–4.80682+2	1.69025+3	IV

Name: Piperidine
Formula: $C_5H_{11}N$

CAS–RN: 110–89–4
Group No.: 33–012
Molar Mass: 85.15

TABLE 33.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
00LOU	N	331.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
34RAD/JUL		290.1	1	nosp	not specified		C_p	BSIO	49WEI
36KUR/VOS	N	311.1	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
64MOE/THO		297.4–327.3	4	0.50	not specified		C_p	BSIO	64MOE/THO
76CON/GIA		298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
88MES/TOD	N	267.3–361.9	12	0.05	99.941	melpt	C_{sat}	BSAO	47HUF
92LAI/ROD		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

00LOU average value in temperature range 293–371 K
36KUR/VOS average value in temperature range 290–333 K
88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

TABLE 33.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88MES/TOD	267.3–361.9	12	0.05	0.722	7.95–3	0.04	6.52–6	–1
				Rejected data				
00LOU	(2.25–1, 1.00, 2.25–1, 1)			34RAD/JUL	(9.90–1, 4.82,–9.90–1, –1)			
36KUR/VOS	(6.04–1, 2.70, 6.04–1, 1)			64MOE/THO	(4.72–1, 2.11, 4.66–1, 4)			
76CON/GIA	(2.13–1, 0.97, 2.13–1, 1)			92LAI/ROD	(2.64–1, 1.24, –2.64–1, –1)			

TABLE 33.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	12	0.834	9.17–3	0.04	6.52–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
267.3–361.9		3.25271+1	–8.47420	1.61606			II

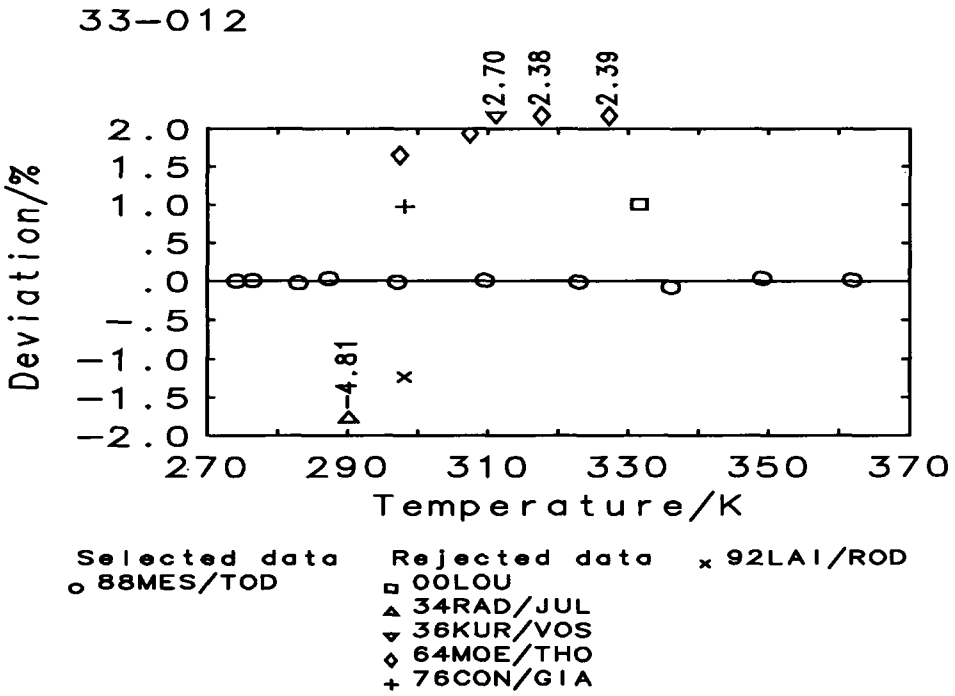
TABLE 33.12.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} ($J\,K^{-1}g^{-1}$)	2.092	2.093	2.096	2.104	2.112	2.114	2.127
C_{sat} ($J\,K^{-1}mol^{-1}$)	178.2	178.2	178.5	179.1	179.8	180.0	181.2
Temp. (K)	320	330	340	350	360		
c_{sat} ($J\,K^{-1}g^{-1}$)	2.144	2.164	2.187	2.213	2.242		
C_{sat} ($J\,K^{-1}mol^{-1}$)	182.6	184.3	186.2	188.4	190.9		

TABLE 33.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	12	1.631	1.80–2	0.08	2.00–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
267.3–361.9	594.00	4.14178+1	1.53321+1	5.69023	2.79713+1	II



Name: 2–Methylpyridine
Formula: C_6H_7N

CAS–RN: 109–06–8
Group No.: 33–013
Molar Mass: 93.13

TABLE 33.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
01KAH	N	346.1	1	nosp	not specified		C_{avg}	DSIO	01KAH
63SCO/HUB		209.9–369.0	19	0.20	99.9	melpt	C_{sat}	BSAO	47HUF

01KAH average value in temperature range 295–397 K

TABLE 33.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
63SCO/HUB	209.9–369.0	19	0.20	0.192	7.52–3	0.04	3.82–6	0
				Rejected data				
01KAH	(2.55–1, 1.25,–2.55–1, –1)							

TABLE 33.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	19	0.216	8.46–3	0.04	3.82–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
209.9–369.0		2.46458+1	–1.00948+1	3.86010	–3.70122–1		II

TABLE 33.13.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.522	1.534	1.549	1.566	1.585	1.606	1.629
C_{sat} (J K^{-1}mol^{-1})	141.7	142.8	144.2	145.8	147.6	149.6	151.7
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.636	1.653	1.679	1.701	1.706	1.734	1.763
C_{sat} (J K^{-1}mol^{-1})	152.4	154.0	156.4	158.4	158.9	161.5	164.1
Temp. (K)	330	340	350	360	370		
c_{sat} (J K^{-1}g^{-1})	1.792	1.821	1.851	1.881	1.910		
C_{sat} (J K^{-1}mol^{-1})	166.9	169.6	172.4	175.1	177.9		

TABLE 33.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	19	1.444	5.40–2	0.29	2.52–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
209.9–369.0	621.00	–3.05330	2.91716	1.10401+1	7.98947–1		II

Name: 3–Methylpyridine
Formula: C_6H_7N

CAS–RN: 108–99–6
Group No.: 33–014
Molar Mass: 93.13

TABLE 33.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63SCO/GOO	257.5–387.9	16	0.20	99.88	melpt	C_{sat}	BSAO	47HUF

TABLE 33.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.106	4.21–3	0.02	3.58–7	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
257.5–387.9		2.34679+1	–8.29377	3.13801	–2.84733–1		II

TABLE 33.14.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.617	1.638	1.645	1.660	1.684	1.704	1.709
C_{sat} (J K^{-1}mol^{-1})	150.6	152.5	153.2	154.6	156.8	158.7	159.1
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	1.735	1.762	1.789	1.817	1.846	1.874	1.903
C_{sat} (J K^{-1}mol^{-1})	161.6	164.1	166.6	169.2	171.9	174.6	177.2
Temp. (K)	380	390					
c_{sat} (J K^{-1}g^{-1})	1.932	1.961					
C_{sat} (J K^{-1}mol^{-1})	179.9	182.6					

TABLE 33.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.535	2.11–2	0.11	3.81–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
257.5–387.9	645.00	–4.62715	8.27955–1	1.17090+1	6.46488		II

Name: 4-Methylpyridine
Formula: C_6H_7N

CAS-RN: 108-89-4
Group No.: 33-015
Molar Mass: 93.13

TABLE 33.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88MES/TOD	N	283.2–394.8	16	0.05	99.967	melpt	C_{sat}	BSAO	47HUF

88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

TABLE 33.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.500	5.20–3	0.03	2.15–6	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
283.1–394.9		1.86409+1	–3.62477	1.64165	–1.24755–1		II

TABLE 33.15.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.663	1.687	1.707	1.712	1.738	1.765	1.792
C_{sat} (J K^{-1}mol^{-1})	154.8	157.1	159.0	159.4	161.8	164.3	166.9
Temp. (K)	340	350	360	370	380	390	
c_{sat} (J K^{-1}g^{-1})	1.820	1.849	1.879	1.909	1.940	1.971	
C_{sat} (J K^{-1}mol^{-1})	169.5	172.2	175.0	177.8	180.6	183.5	

TABLE 33.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.839	8.35–3	0.04	5.48–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
283.1–394.9	646.00	–4.42940	5.75819–1	1.13815+1	8.51813		II

Name: 2,4–Dimethyl–1*H*–pyrrole
Formula: C_6H_9N

CAS–RN: 625–82–1
Group No.: 33–016
Molar Mass: 95.14

TABLE 33.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86STE/CHI	268.4–450.0	22S	nosp	99.979	melpt	C_{sat}	BSAO	47HUF

TABLE 33.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.487	1.21–2	0.05	8.50–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
268.4–450.0		7.80010	4.45322	5.49857–1	–1.06979–1		II

TABLE 33.16.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.899	1.913	1.943	1.986	2.021	2.029	2.071
C_{sat} (J K^{-1}mol^{-1})	180.6	182.0	184.8	189.0	192.3	193.1	197.1
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.113	2.153	2.193	2.231	2.269	2.306	2.341
C_{sat} (J K^{-1}mol^{-1})	201.0	204.9	208.6	212.3	215.9	219.4	222.8
Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	2.376	2.409	2.441	2.471	2.500	2.528	2.554
C_{sat} (J K^{-1}mol^{-1})	226.0	229.2	232.2	235.1	237.9	240.5	243.0

TABLE 33.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.516	1.27–2	0.05	1.36–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
268.4–450.0	671.00	1.63581+1	1.14390	4.69992	5.84814+1		II

Name: 2,5–Dimethyl–1*H*–pyrrole
Formula: C_6H_9N

CAS–RN: 625–84–3
Group No.: 33–017
Molar Mass: 95.14

TABLE 33.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88MES/TOD	N	285.1–383.9	19	0.05	99.89	melpt	C_{sat}	BSAO	47HUF

88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

TABLE 33.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.406	5.10–3	0.02	2.41–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
285.1–383.9		1.41426+1	–2.18561	2.85540	–3.58939–1		II

TABLE 33.17.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	2.016	2.053	2.062	2.107	2.152	2.196	2.238
C_{sat} (J K^{-1}mol^{-1})	191.8	195.4	196.2	200.5	204.8	208.9	213.0
Temp. (K)	350	360	370	380			
c_{sat} (J K^{-1}g^{-1})	2.279	2.319	2.356	2.392			
C_{sat} (J K^{-1}mol^{-1})	216.9	220.6	224.2	227.6			

TABLE 33.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.601	7.35–3	0.03	4.22–6	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
285.1–383.9	671.00	2.55874+1	2.19081	1.39318	7.47116+1		II

Name: 1,4–Diazobicyclo[2.2.2]octane
Formula: $C_6H_{12}N_2$

CAS–RN: 280–57–9
Group No.: 33–018
Molar Mass: 112.17

TABLE 33.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
63TRO/WES	433.7–448.0	12	0.08	99.997	melpt	C_{sat}	BSAO	53WES/HAT

TABLE 33.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	1.962	4.53–2	0.16	1.19–4	2
Temp. range K		A_1	A_2				Level of uncertainty
433.7–448.0		7.78019	4.84508				II

TABLE 33.18.4. Recommended values of heat capacities

Temp. (K)	435	440	445	450
c_{sat} (J K^{-1}g^{-1})	2.139	2.157	2.175	2.193
C_{sat} (J K^{-1}mol^{-1})	239.9	241.9	244.0	246.0

Name: Hexahydro-1*H*-azepine
Formula: $C_6H_{13}N$

CAS-RN: 111-49-9
Group No.: 33-019
Molar Mass: 99.18

TABLE 33.19.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CON/GIA	298.15	2.067	nosp	not specified		C_p	BDCT	76CON/GIA

Name: 1-Methylpiperidine
Formula: $C_6H_{13}N$

CAS-RN: 626-67-5
Group No.: 33-020
Molar Mass: 99.18

TABLE 33.20.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CON/GIA	298.15	1.865	nosp	not specified		C_p	BDCT	76CON/GIA

Name: 2-Methylpiperidine
Formula: $C_6H_{13}N$

CAS-RN: 109-05-7
Group No.: 33-021
Molar Mass: 99.18

TABLE 33.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CON/GIA		298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
88MES/TOD	N	273.2-369.8	13	0.05	99.87	melpt	C_{sat}	BSAO	47HUF

88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

TABLE 33.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
88MES/TOD	273.2-369.8	13	0.05	0.414	5.34-3	0.02	2.20-6	-1
				Rejected data				
76CON/GIA	(9.52-1, 3.86,-9.52-1, -1)							

TABLE 33.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	13	0.498	6.42–3	0.02	2.20–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
273.2–369.8		7.23059+1	–3.95422+1	1.04706+1	–8.25468–1		II

TABLE 33.21.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.148	2.146	2.143	2.143	2.147	2.148	2.159
C_{sat} (J K^{-1}mol^{-1})	213.1	212.8	212.5	212.5	212.9	213.1	214.2
Temp. (K)	320	330	340	350	360	370	
c_{sat} (J K^{-1}g^{-1})	2.175	2.195	2.218	2.245	2.275	2.308	
C_{sat} (J K^{-1}mol^{-1})	215.7	217.6	220.0	222.7	225.7	228.9	

TABLE 33.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	10	3.257	4.26–2	0.16	9.15–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
285.4–369.8	598.00	5.40853+1	1.94914+1	5.38516	3.75193+1		II

Name: 4–Methylpiperidine
Formula: $C_6H_{13}N$

CAS–RN: 626–58–4
Group No.: 33–022
Molar Mass: 99.18

TABLE 33.22.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76CON/GIA	298.15	2.109	nosp	not specified		C_p	BDCT	76CON/GIA

Name: 1–Piperazineethanamine
Formula: $C_6H_{15}N_3$

CAS–RN: 140–31–8
Group No.: 33–023
Molar Mass: 129.21

TABLE 33.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88BOB/KAM	333.1–473.1	8	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 33.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.149	3.45–1	0.89	3.91–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
333.1–473.1		4.49974+1	–9.07402	1.74053			VI

TABLE 33.23.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	2.19	2.21	2.22	2.25	2.27	2.29	2.32
C_{sat} (J K^{-1}mol^{-1})	283	285	287	290	293	296	300
Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	2.35	2.38	2.42	2.46	2.49	2.54	2.58
C_{sat} (J K^{-1}mol^{-1})	304	308	313	317	322	328	333
Temp. (K)	470						
c_{sat} (J K^{-1}g^{-1})	2.63						
C_{sat} (J K^{-1}mol^{-1})	339						

TABLE 33.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.144	3.28–1	0.86	3.56–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
333.1–473.1	707.00	2.83327	7.35627	2.18179+1	2.72808–1		VI

Name: 2,3–Dimethylpyridine
Formula: C_7H_9N

CAS–RN: 583–61–9
Group No.: 33–024
Molar Mass: 107.16

TABLE 33.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86STE/CHI	258.6–450.0	23S	nosp	99.86	melpt	C_{sat}	BSAO	47HUF

TABLE 33.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	23	0.256	6.59–3	0.03	3.98–6	0
C_{sat}	23	23	0.245	6.29–3	0.02	1.99–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
258.6–450.0	2.32557+1	–5.06808	2.15349	–1.69356–1	II
258.6–450.0	2.37483+1	–5.54745	2.30763	–1.85729–1	II

TABLE 33.24.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.681	1.702	1.709	1.725	1.749	1.769	1.774
C_p ($J K^{-1} mol^{-1}$)	180.1	182.4	183.2	184.8	187.4	189.6	190.1
c_{sat} ($J K^{-1} g^{-1}$)	1.681	1.702	1.709	1.725	1.749	1.769	1.774
C_{sat} ($J K^{-1} mol^{-1}$)	180.1	182.4	183.1	184.8	187.4	189.6	190.1
Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.800	1.827	1.854	1.883	1.912	1.941	1.971
C_p ($J K^{-1} mol^{-1}$)	192.8	195.7	198.7	201.7	204.8	208.0	211.2
c_{sat} ($J K^{-1} g^{-1}$)	1.800	1.827	1.854	1.883	1.912	1.941	1.971
C_{sat} ($J K^{-1} mol^{-1}$)	192.9	195.7	198.7	201.7	204.8	208.0	211.2
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.002	2.033	2.064	2.095	2.127	2.158	2.190
C_p ($J K^{-1} mol^{-1}$)	214.5	217.8	221.2	224.5	227.9	231.3	234.6
c_{sat} ($J K^{-1} g^{-1}$)	2.002	2.033	2.064	2.095	2.126	2.157	2.188
C_{sat} ($J K^{-1} mol^{-1}$)	214.5	217.8	221.1	224.4	227.8	231.1	234.4
Temp. (K)	450						
c_p ($J K^{-1} g^{-1}$)	2.221						
C_p ($J K^{-1} mol^{-1}$)	238.0						
c_{sat} ($J K^{-1} g^{-1}$)	2.218						
C_{sat} ($J K^{-1} mol^{-1}$)	237.7						

TABLE 33.24.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	23	1.791	4.46–2	0.18	1.51–4	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
258.6–450.0	655.40	–4.49183	4.13926–1	1.38146+1	1.21861+1	II

Name: 2,4-Dimethylpyridine
Formula: C_7H_9N

CAS-RN: 108-47-4
Group No.: 33-025
Molar Mass: 107.16

TABLE 33.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86STE/CHI	209.4–450.0	28S	nosp	99.44	melpt	C_{sat}	BSAO	47HUF

TABLE 33.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	28	28	0.508	1.17–2	0.05	7.49–6	5
C_{sat}	28	28	0.469	1.08–2	0.05	5.72–6	5

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
209.4–450.0	2.42219+1	–6.76773	2.70673	–2.22736–1	II
209.4–450.0	2.44573+1	–7.02415	2.79796	–2.33342–1	II

TABLE 33.25.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1}g^{-1}$)	1.543	1.557	1.572	1.590	1.609	1.630	1.653
C_p ($J K^{-1}mol^{-1}$)	165.3	166.8	168.5	170.4	172.4	174.7	177.1
c_{sat} ($J K^{-1}g^{-1}$)	1.543	1.557	1.572	1.590	1.609	1.630	1.652
C_{sat} ($J K^{-1}mol^{-1}$)	165.3	166.8	168.5	170.4	172.4	174.7	177.1
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	1.660	1.676	1.701	1.723	1.728	1.755	1.783
C_p ($J K^{-1}mol^{-1}$)	177.9	179.6	182.3	184.6	185.1	188.1	191.1
c_{sat} ($J K^{-1}g^{-1}$)	1.660	1.676	1.701	1.723	1.728	1.755	1.783
C_{sat} ($J K^{-1}mol^{-1}$)	177.9	179.6	182.3	184.6	185.1	188.1	191.1
Temp. (K)	330	340	350	360	370	380	390
c_p ($J K^{-1}g^{-1}$)	1.813	1.843	1.873	1.905	1.936	1.968	2.001
C_p ($J K^{-1}mol^{-1}$)	194.2	197.4	200.7	204.1	207.5	210.9	214.4
c_{sat} ($J K^{-1}g^{-1}$)	1.813	1.843	1.873	1.905	1.936	1.968	2.000
C_{sat} ($J K^{-1}mol^{-1}$)	194.2	197.5	200.7	204.1	207.5	210.9	214.3
Temp. (K)	400	410	420	430	440	450	
c_p ($J K^{-1}g^{-1}$)	2.033	2.066	2.098	2.131	2.163	2.194	
C_p ($J K^{-1}mol^{-1}$)	217.9	221.4	224.8	228.3	231.7	235.1	
c_{sat} ($J K^{-1}g^{-1}$)	2.032	2.065	2.097	2.129	2.160	2.192	
C_{sat} ($J K^{-1}mol^{-1}$)	217.8	221.2	224.7	228.1	231.5	234.8	

TABLE 33.25.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	28	28	1.191	2.73–2	0.12	4.35–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
209.4–450.0	647.00	7.31883+1	4.89103	1.35751+1	6.83058+1	3.05744+1	6.93846+1	II

Name: 2,5–Dimethylpyridine
Formula: C_7H_9N

CAS–RN: 589–93–5
Group No.: 33–026
Molar Mass: 107.16

TABLE 33.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86STE/CHI	259.1–450.0	23S	nosp	99.64	melpt	C_{sat}	BSAO	47HUF

TABLE 33.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	23	0.157	3.90–3	0.02	1.41–6	–1
C_{sat}	23	23	0.150	3.81–3	0.02	6.63–7	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
259.1–450.0	2.32355+1	–5.83663	2.43956	–2.00038–1	II
259.1–450.0	2.37250+1	–6.31800	2.59619	–2.16894–1	II

TABLE 33.26.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.632	1.655	1.662	1.678	1.703	1.724	1.729
C_p (J K^{-1}mol^{-1})	174.9	177.3	178.1	179.8	182.5	184.7	185.3
c_{sat} (J K^{-1}g^{-1})	1.632	1.655	1.662	1.678	1.703	1.724	1.729
C_{sat} (J K^{-1}mol^{-1})	174.9	177.3	178.1	179.8	182.5	184.7	185.3
Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.756	1.783	1.812	1.841	1.871	1.902	1.932
C_p (J K^{-1}mol^{-1})	188.1	191.1	194.2	197.3	200.5	203.8	207.1
c_{sat} (J K^{-1}g^{-1})	1.756	1.783	1.812	1.841	1.871	1.902	1.932
C_{sat} (J K^{-1}mol^{-1})	188.1	191.1	194.2	197.3	200.5	203.8	207.1
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	1.964	1.995	2.027	2.058	2.090	2.121	2.153
C_p (J K^{-1}mol^{-1})	210.4	213.8	217.2	220.6	224.0	227.3	230.7
c_{sat} (J K^{-1}g^{-1})	1.963	1.995	2.026	2.057	2.089	2.120	2.150
C_{sat} (J K^{-1}mol^{-1})	210.4	213.7	217.1	220.5	223.8	227.1	230.4
Temp. (K)	450						
c_p (J K^{-1}g^{-1})	2.184						
C_p (J K^{-1}mol^{-1})	234.0						
c_{sat} (J K^{-1}g^{-1})	2.181						
C_{sat} (J K^{-1}mol^{-1})	233.7						

TABLE 33.26.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	23	0.321	7.55–3	0.03	4.64–6	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
259.1–450.0	644.20	3.72561+1	2.10117	1.53743+1	3.65064+1	2.67448+1	3.49453+1	II

Name: 2,6–Dimethylpyridine
Formula: C_7H_9N

CAS–RN: 108–48–5
Group No.: 33–027
Molar Mass: 107.16

TABLE 33.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86STE/CHI	267.0–440.0	21S	nosp	99.884	melpt	C_{sat}	BSAO	47HUF

TABLE 33.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	21	0.271	6.21–3	0.03	2.27–6	2
C_{sat}	21	21	0.264	6.05–3	0.03	1.63–6	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
267.0–440.0	1.93830+1	–2.87123	1.67178	–1.28623–1	II
267.0–440.0	1.99925+1	–3.47319	1.86892	–1.50026–1	II

TABLE 33.27.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.652	1.660	1.678	1.705	1.728	1.734	1.763
C_p (J K^{-1}mol^{-1})	177.0	177.9	179.8	182.7	185.2	185.8	188.9
c_{sat} (J K^{-1}g^{-1})	1.652	1.660	1.678	1.705	1.728	1.734	1.763
C_{sat} (J K^{-1}mol^{-1})	177.0	177.9	179.8	182.7	185.2	185.8	188.9

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.792	1.823	1.854	1.885	1.917	1.950	1.983
C_p (J K^{-1}mol^{-1})	192.1	195.3	198.6	202.0	205.5	209.0	212.5
c_{sat} (J K^{-1}g^{-1})	1.792	1.823	1.854	1.885	1.917	1.950	1.982
C_{sat} (J K^{-1}mol^{-1})	192.1	195.3	198.6	202.0	205.5	208.9	212.4

Temp. (K)	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.016	2.050	2.083	2.117	2.151	2.185
C_p (J K^{-1}mol^{-1})	216.0	219.6	223.2	226.9	230.5	234.1
c_{sat} (J K^{-1}g^{-1})	2.015	2.049	2.082	2.115	2.148	2.181
C_{sat} (J K^{-1}mol^{-1})	216.0	219.5	223.1	226.6	230.2	233.7

TABLE 33.27.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	21	0.347	7.95–3	0.03	3.82–6	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
267.0–440.0	623.80	1.39683+1	5.32466–1	1.51920+1	1.89273+1	1.99693+1	1.40752+1	II

Name: 3,4–Dimethylpyridine
Formula: C_7H_9N

CAS–RN: 583–58–4
Group No.: 33–028
Molar Mass: 107.16

TABLE 33.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
84POD/RAC	N	264.6–378.0	76	1.00	not specified		C_{sat}	BSAO	84POD/RAC
86STE/CHI		262.7–450.0	22S	nosp	99.71	melpt	C_{sat}	BSAO	47HUF

84POD/RAC only a graph given in the paper; experimental values provided by the author

TABLE 33.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86STE/CHI	262.7–450.0	22	0.10#	0.197	4.87–3	0.02	1.91–6	–1
				Rejected data				
84POD/RAC	(3.99–1, 1.64, 2.74–1, 60)							

TABLE 33.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	98	22	0.218	5.39–3	0.02	1.91–6	–1

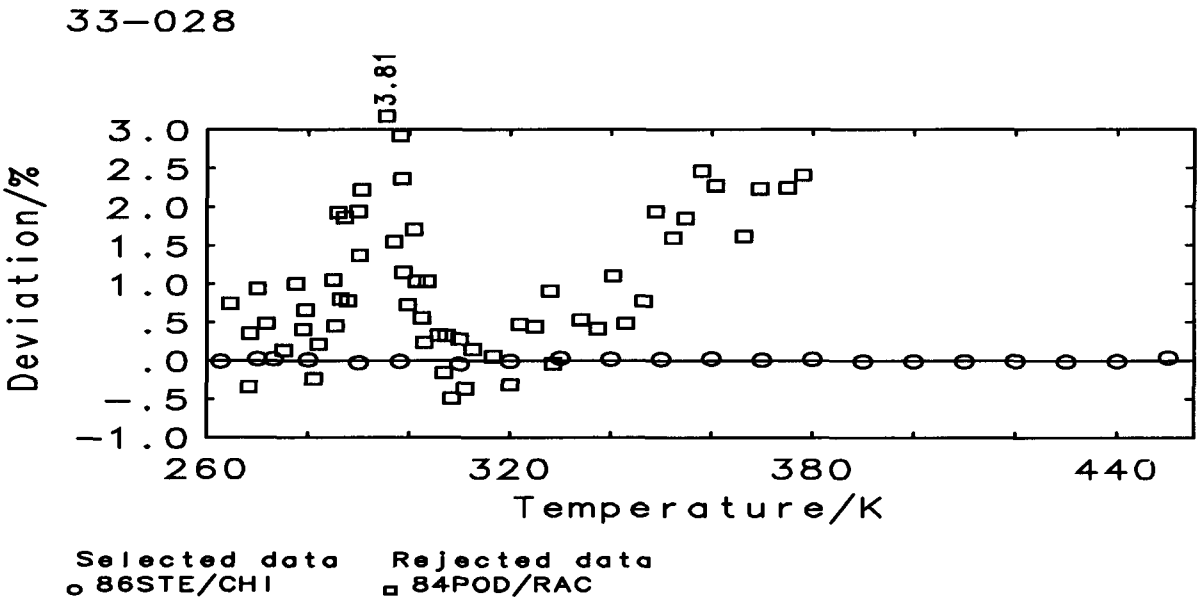
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
262.7–450.0	2.69180+1	–7.43794	2.72072	–2.20795–1	II

TABLE 33.28.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.732	1.738	1.752	1.773	1.790	1.795	1.818
C_{sat} (J K^{-1}mol^{-1})	185.6	186.3	187.7	189.9	191.9	192.3	194.8
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	1.842	1.867	1.893	1.920	1.948	1.976	2.004
C_{sat} (J K^{-1}mol^{-1})	197.4	200.1	202.9	205.8	208.7	211.7	214.7
Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	2.033	2.061	2.090	2.119	2.148	2.177	2.205
C_{sat} (J K^{-1}mol^{-1})	217.8	220.9	224.0	227.1	230.2	233.3	236.3

TABLE 33.28.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	98	22	0.396	9.94–3	0.04	4.94–6	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
262.7–450.0	683.80	8.09102+1	5.76083	1.40774+1	7.51494+1	3.46420+1	6.96899+1	II



Name: 3,5–Dimethylpyridine
Formula: C_7H_9N

CAS–RN: 591–22–0
Group No.: 33–029
Molar Mass: 107.16

TABLE 33.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86STE/CHI	266.8–450.0	22S	nosp	99.812	melpt	C_{sat}	BSAO	47HUF

TABLE 33.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.159	3.73–3	0.02	–4.33–7	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
266.8–450.0	2.18007+1	–4.44272	2.00122	–1.56328–1	II

TABLE 33.29.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.654	1.661	1.677	1.702	1.723	1.727	1.754
C_{sat} (J K^{-1}mol^{-1})	177.2	178.0	179.8	182.4	184.6	185.1	187.9
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	1.781	1.809	1.838	1.867	1.897	1.927	1.958
C_{sat} (J K^{-1}mol^{-1})	190.9	193.9	196.9	200.1	203.3	206.5	209.8
Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	1.989	2.021	2.052	2.084	2.116	2.148	2.179
C_{sat} (J K^{-1}mol^{-1})	213.2	216.5	219.9	223.3	226.7	230.1	233.5

TABLE 33.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.280	6.69–3	0.03	1.30–6	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
266.8–450.0	667.20	3.41115+1	1.87271	1.52831+1	3.46167+1	2.78038+1	3.04189+1	II

Name: Octahydroazocine
Formula: $C_7H_{15}N$

CAS–RN: 1121–92–2
Group No.: 33–030
Molar Mass: 113.20

TABLE 33.30.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CON/GIA	298.15	2.033	nosp	not specified		C_p	BDCT	76CON/GIA

Name: 2,3,6-Trimethylpyridine
Formula: $C_8H_{11}N$

CAS–RN: 1462–84–6
Group No.: 33–031
Molar Mass: 121.18

TABLE 33.31.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91SVO/ZAB1	300.6–328.4	7	0.30	99.9	chrom	C_p	BSAO	91SVO/ZAB1

TABLE 33.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.218	1.79–2	0.07	9.26–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
300.6–328.4		4.95763+1	−1.83653+1	3.55085			III

TABLE 33.31.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.814	1.837	1.864	1.896
C_p ($J K^{-1} mol^{-1}$)	219.8	222.6	225.9	229.8

Name: 2,4,6–Trimethylpyridine
Formula: $C_8H_{11}N$

CAS–RN: 108–75–8
Group No.: 33–032
Molar Mass: 121.18

TABLE 33.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91SVO/ZAB1	300.6–328.4	7	0.30	99.9	chrom	C_p	BSAO	91SVO/ZAB1

TABLE 33.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.669	5.28–2	0.20	1.63–4	−1
Temp. range K		A_1	A_2				Level of uncertainty
300.6–328.4		9.82856	5.31204				III

TABLE 33.32.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p ($J K^{-1}g^{-1}$)	1.768	1.804	1.841	1.877
C_p ($J K^{-1}mol^{-1}$)	214.2	218.6	223.1	227.5

Name: 3–Azabicyclo[3.2.2]nonane
Formula: $C_8H_{15}N$

CAS–RN: 283–24–9
Group No.: 33–033
Molar Mass: 125.21

TABLE 33.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64WUL/WES	470.9–489.4	5	nosp	99.79	melpt	C_p	BSAO	53WES/HAT

TABLE 33.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.799	8.85–2	0.24	2.54–4	–1

Temp. range K	A_1	A_2	Level of uncertainty
470.9–489.4	6.24899	6.39181	III

TABLE 33.33.4. Recommended values of heat capacities

Temp. (K)	470	480	490
c_p ($J K^{-1}g^{-1}$)	2.410	2.452	2.495
C_p ($J K^{-1}mol^{-1}$)	301.7	307.1	312.4

Name: 1,4–Piperazinediethanamine
Formula: $C_8H_{20}N_4$

CAS–RN: 6531–38–0
Group No.: 33–034
Molar Mass: 172.27

TABLE 33.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	333.1–473.1	8	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 33.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.293	9.41–1	1.76	2.15–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
333.1–473.1		8.57798+1	–2.31392+1	3.70559			VI

TABLE 33.34.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	2.40	2.41	2.42	2.44	2.46	2.48	2.50
C_{sat} (J K^{-1}mol^{-1})	414	415	417	420	423	427	432
Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	2.53	2.57	2.60	2.64	2.69	2.74	2.79
C_{sat} (J K^{-1}mol^{-1})	437	442	449	456	463	471	480
Temp. (K)	470						
c_{sat} (J K^{-1}g^{-1})	2.84						
C_{sat} (J K^{-1}mol^{-1})	490						

Name: *N*–[2–(1–Piperazinyl)ethyl]–1,2–ethanediamine
Formula: $C_8H_{20}N_4$

CAS–RN: 24028–46–4
Group No.: 33–035
Molar Mass: 172.27

TABLE 33.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88BOB/KAM	333.1–473.1	8	6.00	97.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 33.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.129	3.74–1	0.77	3.72–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
333.1–473.1		–6.69007	2.29253+1	–2.07378			VI

TABLE 33.35.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	2.24	2.28	2.32	2.36	2.40	2.44	2.47
C_{sat} (J K^{-1}mol^{-1})	386	393	400	407	414	420	426
Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	2.50	2.53	2.56	2.58	2.61	2.63	2.65
C_{sat} (J K^{-1}mol^{-1})	431	436	441	445	449	453	456
Temp. (K)	470						
c_{sat} (J K^{-1}g^{-1})	2.67						
C_{sat} (J K^{-1}mol^{-1})	459						

Name: Isoquinoline
Formula: C_9H_7N

CAS–RN: 119–65–3
Group No.: 33–036
Molar Mass: 129.16

TABLE 33.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88STE/ARC N	299.6–400.0	12S	0.10	99.991	melpt	C_{sat}	BSAO	47HUF

88STE/ARC same data in 86STE/CHI

TABLE 33.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.308	7.75–3	0.03	4.61–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
299.6–400.0		3.14368+1	–1.30334+1	4.79389	–4.37707–1		II

TABLE 33.36.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_{sat} (J K^{-1}g^{-1})	1.523	1.549	1.576	1.603	1.631	1.659	1.688
C_{sat} (J K^{-1}mol^{-1})	196.8	200.1	203.5	207.0	210.7	214.3	218.0
Temp. (K)	370	380	390	400			
c_{sat} (J K^{-1}g^{-1})	1.717	1.746	1.774	1.802			
C_{sat} (J K^{-1}mol^{-1})	221.8	225.5	229.1	232.7			

TABLE 33.36.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.592	1.49–2	0.06	1.33–5	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
299.6–400.0	803.00	–6.99717	5.92604–1	1.17181+1	2.06548+1	II

Name: Quinoline
Formula: C_9H_7N

CAS–RN: 91–22–5
Group No.: 33–037
Molar Mass: 129.16

TABLE 33.37.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
16BRA		283.1	1	nosp	not specified		C_{avg}	DSTO	16BRA
34KOL/UDO2	N	302.4	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
34RAD/JUL		289.6	1	nosp	not specified		C_p	BSIO	49WEI
36PAR/TOD1		260.0–300.0	5S	0.70	not specified		C_p	BSIO	25PAR
47PUS/FED		287.9–305.0	4	nosp	not specified		C_p	DSIO	47PUS/FED
51TSC/KRI		298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
88STE/ARC	N	258.4–450.0	23S	0.10	99.985	melpt	C_{sat}	BSAO	47HUF
90JAL/ROB		293.0	1	5.00	99.	anal	C_p	BDHT	87PER/COM

34KOL/UDO2 same datum in 34KOL/UDO1
88STE/ARC similar data in 86STE/CHI

TABLE 33.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88STE/ARC	258.4–450.0	23	0.10	0.240	6.41–3	0.02	1.74–6	0
				Rejected data				
16BRA	(7.89–2, 0.34, 7.89–2, 1)			34KOL/UDO2	(4.19–1, 1.81,–4.19–1, –1)			
34RAD/JUL	(3.28, 16.57, –3.28, –1)			36PAR/TOD1	(3.82–1, 1.63, 3.62–1, 5)			
47PUS/FED	(3.98–1, 1.73,–3.95–1, –4)			51TSC/KRI	(1.06, 4.32, 1.06, 1)			
90JAL/ROB	(7.56–2, 0.33,–7.56–2, –1)							

TABLE 33.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	37	23	0.264	7.05–3	0.03	1.74–6	0

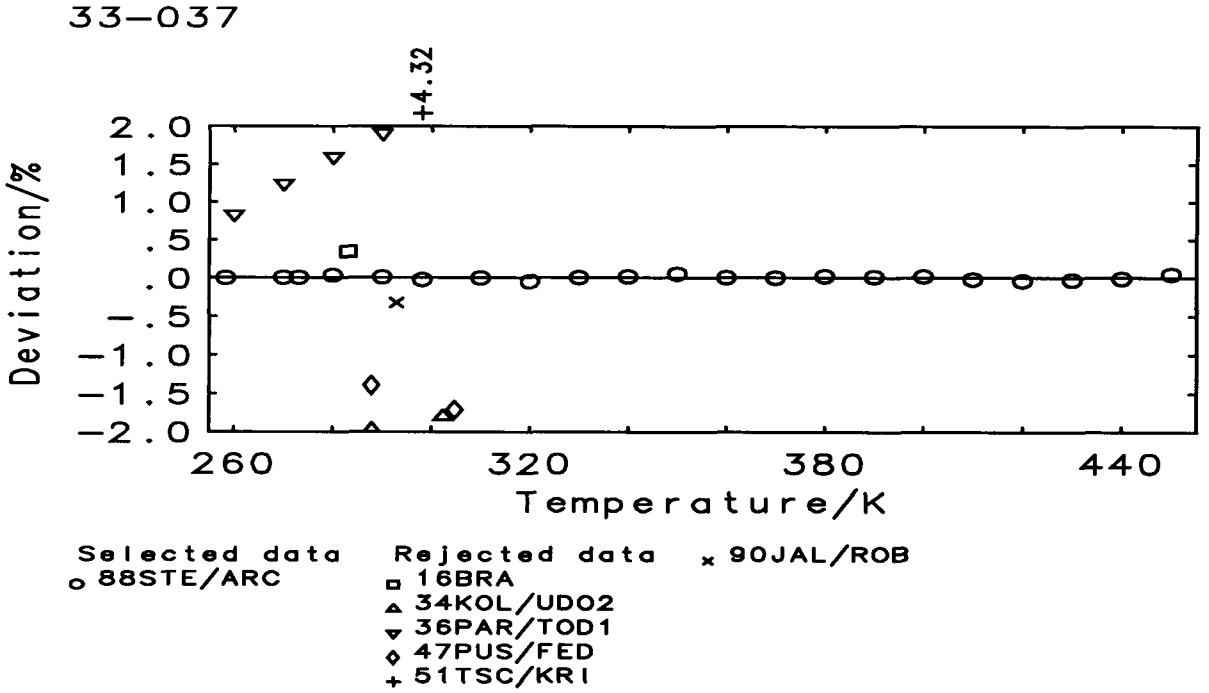
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
258.4–450.0	1.75664+1	–1.88265	1.78689	–1.65720–1	II

TABLE 33.37.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} ($J\,K^{-1}g^{-1}$)	1.406	1.432	1.441	1.459	1.487	1.509	1.514
C_{sat} ($J\,K^{-1}mol^{-1}$)	181.6	185.0	186.1	188.5	192.0	194.9	195.6
Temp. (K)	310	320	330	340	350	360	370
c_{sat} ($J\,K^{-1}g^{-1}$)	1.543	1.571	1.600	1.629	1.658	1.688	1.717
C_{sat} ($J\,K^{-1}mol^{-1}$)	199.3	203.0	206.7	210.4	214.2	218.0	221.7
Temp. (K)	380	390	400	410	420	430	440
c_{sat} ($J\,K^{-1}g^{-1}$)	1.746	1.775	1.804	1.832	1.861	1.888	1.916
C_{sat} ($J\,K^{-1}mol^{-1}$)	225.5	229.2	233.0	236.7	240.3	243.9	247.4
Temp. (K)	450						
c_{sat} ($J\,K^{-1}g^{-1}$)	1.943						
C_{sat} ($J\,K^{-1}mol^{-1}$)	250.9						

TABLE 33.37.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	37	23	1.144	2.91–2	0.11	7.53–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
258.4–450.0	782.00	–1.53517	1.85359–2	1.05881+1	3.17863+1		II



Name: 1,2,3,4–Tetrahydroquinoline
Formula: $C_9H_{11}N$

CAS–RN: 635–46–1
Group No.: 33–038
Molar Mass: 133.19

TABLE 33.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI2	298.0–441.3	16	0.10	99.956	melpt	C_{sat}	BSAO	47HUF

TABLE 33.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.353	1.08–2	0.04	5.96–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.0–441.3		1.58925+1	3.82469	1.24145–1			II

TABLE 33.38.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_{sat} (J K^{-1}g^{-1})	1.778	1.807	1.835	1.864	1.893	1.923	1.952
C_{sat} (J K^{-1}mol^{-1})	236.8	240.6	244.5	248.3	252.2	256.1	260.0
Temp. (K)	370	380	390	400	410	420	430
c_{sat} (J K^{-1}g^{-1})	1.982	2.011	2.041	2.071	2.101	2.132	2.162
C_{sat} (J K^{-1}mol^{-1})	263.9	267.9	271.9	275.9	279.9	283.9	288.0
Temp. (K)	440						
c_{sat} (J K^{-1}g^{-1})	2.193						
C_{sat} (J K^{-1}mol^{-1})	292.0						

TABLE 33.38.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.345	1.05–2	0.03	5.96–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
298.0–441.3	771.00	–3.58786	1.10205–1	1.51719+1	2.92018+1		II

Name: 5,6,7,8–Tetrahydroquinoline
Formula: $C_9H_{11}N$

CAS–RN: 10500–57–9
Group No.: 33–039
Molar Mass: 133.19

TABLE 33.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI2	N	225.9–442.0	28	0.10	99.974	melpt	C_{sat}	BSAO	47HUF

89STE/CHI2 smoothed data in 86STE/CHI

TABLE 33.39.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.199	4.88–3	0.02	1.43–6	2
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
225.9–325.0	2.88292+1	–1.16034+1	5.09997	–5.06556–1			II
325.0–442.0	1.66466+1	–3.57958–1	1.63983	–1.51670–1			II

TABLE 33.39.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.433	1.458	1.484	1.513	1.542	1.552	1.573
C_{sat} (J K^{-1}mol^{-1})	190.9	194.2	197.7	201.5	205.4	206.7	209.6
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.605	1.632	1.638	1.672	1.706	1.740	1.774
C_{sat} (J K^{-1}mol^{-1})	213.8	217.4	218.2	222.7	227.2	231.7	236.3
Temp. (K)	350	360	370	380	390	400	410
c_{sat} (J K^{-1}g^{-1})	1.809	1.844	1.878	1.913	1.947	1.982	2.016
C_{sat} (J K^{-1}mol^{-1})	240.9	245.6	250.2	254.8	259.4	263.9	268.5
Temp. (K)	420	430	440				
c_{sat} (J K^{-1}g^{-1})	2.050	2.083	2.116				
C_{sat} (J K^{-1}mol^{-1})	273.0	277.4	281.9				

TABLE 33.39.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.775	2.08–2	0.08	2.49–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
225.9–442.0	735.00	2.35827+2	2.19914+1	–3.92910	2.17141+2	1.21278+2	1.15775+2	II

Name: 1,1'–(1,2–Ethanediyl)bispiperazine
Formula: $C_{10}H_{22}N_4$

CAS–RN: 19479–83–5
Group No.: 33–040
Molar Mass: 198.31

TABLE 33.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	413.1–473.1	4	6.00	95.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 33.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	0.126	5.23–1	0.75	3.83–3	0
Temp. range K		A_1	A_2				Level of uncertainty
413.1–473.1		1.95959+1	1.09656+1				VI

TABLE 33.40.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440	450	460	470
c_{sat} (J $K^{-1}g^{-1}$)	2.71	2.75	2.80	2.84	2.89	2.94	2.98
C_{sat} (J $K^{-1}mol^{-1}$)	537	546	555	564	573	582	591

Name: *N*–(2–Aminoethyl)–1,4–piperazinediethanamine
Formula: $C_{10}H_{25}N_5$

CAS–RN: 31295–54–2
Group No.: 33–041
Molar Mass: 215.34

TABLE 33.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BOB/KAM	333.1–473.1	8	6.00	95.	chrom	C_{sat}	BDCT	86MER/BEN

TABLE 33.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.063	2.63–1	0.38	8.70–4	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
333.1–473.1		–2.62420+2	2.54637+2	–6.67327+1	5.90829		VI

TABLE 33.41.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	2.45	2.48	2.50	2.51	2.53	2.54	2.55
C_{sat} (J K^{-1}mol^{-1})	528	533	538	541	544	547	550
Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	2.57	2.59	2.61	2.64	2.68	2.72	2.78
C_{sat} (J K^{-1}mol^{-1})	553	557	562	569	576	586	598
Temp. (K)	470						
c_{sat} (J K^{-1}g^{-1})	2.84						
C_{sat} (J K^{-1}mol^{-1})	612						

Name: Acridine
Formula: $C_{13}H_9N$

CAS–RN: 260–94–6
Group No.: 33–042
Molar Mass: 179.22

TABLE 33.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI1	N	391.9–445.5	9	0.10	99.988	melpt	C_{sat}	BSAO	47HUF

89STE/CHI1 smoothed data in 86STE/CHI

TABLE 33.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	8	0.313	1.21–2	0.03	4.77–6	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
393.8–445.5		3.35322	1.14365+1	–6.93552–1			II

TABLE 33.42.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	1.735	1.763	1.790	1.816	1.842	1.867	1.892
C_{sat} (J K^{-1}mol^{-1})	311.0	316.0	320.8	325.5	330.1	334.6	339.0

TABLE 33.42.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	8	0.306	1.18–2	0.03	2.38–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
393.8–445.5	889.90	4.88452+1	4.75622	2.14963	1.25407+2		II

Name: Benzo[*h*]quinoline
Formula: $C_{13}H_9N$

CAS–RN: 230–27–3
Group No.: 33–043
Molar Mass: 179.22

TABLE 33.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI1	327.7–439.6	16	0.10	99.89	melpt	C_{sat}	BSAO	47HUF

TABLE 33.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.102	3.56–3	0.01	–2.38–7	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
327.8–439.6		1.87742+1	6.41582–1	1.60274	–1.55143–1		II

TABLE 33.43.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	1.520	1.549	1.577	1.606	1.634	1.663	1.691
C_{sat} (J K^{-1}mol^{-1})	272.5	277.6	282.7	287.8	292.9	298.0	303.1
Temp. (K)	400	410	420	430	440		
c_{sat} (J K^{-1}g^{-1})	1.719	1.747	1.774	1.802	1.828		
C_{sat} (J K^{-1}mol^{-1})	308.1	313.1	318.0	322.9	327.7		

TABLE 33.43.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.159	5.66–3	0.02	1.91–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
327.8–439.6	884.00	1.01906+1	3.68699–1	1.06544+1	7.04146+1		II

Name: Phenanthridine
Formula: $C_{13}H_9N$

CAS–RN: 229–87–8
Group No.: 33–044
Molar Mass: 179.22

TABLE 33.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI1	N	377.1–439.6	9	0.10	99.975	melpt	C_{sat}	BSAO	47HUF

89STE/CHI1 smoothed data in 86STE/CHI

TABLE 33.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.357	1.34–2	0.04	3.39–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
377.1–439.6		1.52429+1	5.64025				II

TABLE 33.44.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c_{sat} (J K^{-1}g^{-1})	1.701	1.728	1.754	1.780	1.806	1.832	1.858
C_{sat} (J K^{-1}mol^{-1})	304.9	309.6	314.3	319.0	323.7	328.4	333.1

TABLE 33.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.323	1.22–2	0.03	2.97–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
377.1–439.6	911.00	1.12949+1	4.53194–1	1.26325+1	7.03753+1		II

Name: 9–Methyl–9*H*–carbazole
Formula: $C_{13}H_{11}N$

CAS–RN: 1484–12–4
Group No.: 33–045
Molar Mass: 181.24

TABLE 33.45.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88MES/TOD	N	366.1–388.4	8	0.05	99.997	melpt	C_{sat}	BSAO	47HUF
92STE/CHI1		370.0–750.0	20	1.00	99.99	chrom	C_{sat}	BDHT	89KNI/ARC

88MES/TOD same data in 87MES/TOD and smoothed data in 86STE/CHI

TABLE 33.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88MES/TOD	366.1–388.4	8	0.05	0.798	1.51–2	0.04	8.63–5	0
92STE/CHI1	370.0–750.0	20	1.00	0.137	6.66-2	0.14	–1.18-2	–2

TABLE 33.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	28	0.478	6.15–2	0.13	–8.40–3	–2
C_{sat}	28	28	0.484	7.14–2	0.15	–9.99–3	–2

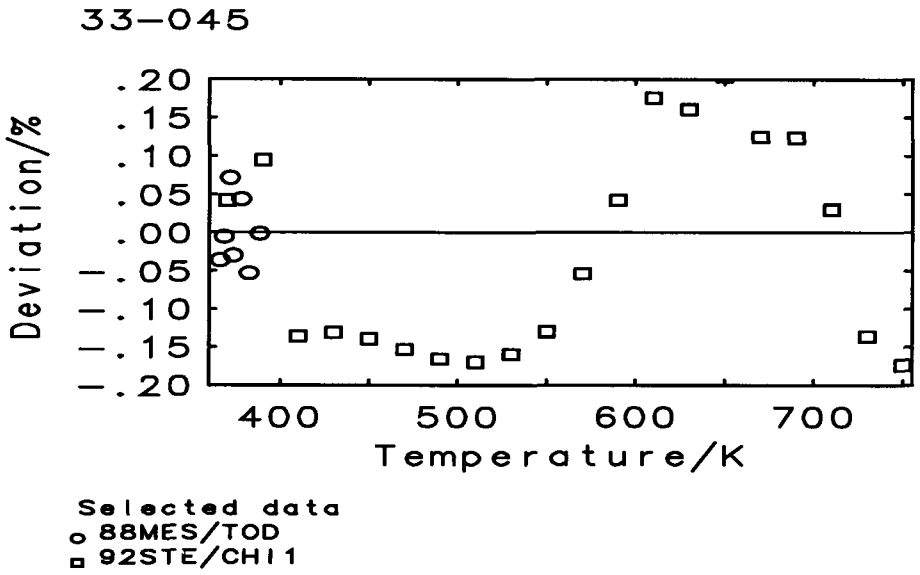
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
366.1–750.0	2.34521+1	1.41477	8.83139–1	–6.30297–2	III
366.1–750.0	2.44972+1	6.81255–1	1.05198	–7.57147–2	III

TABLE 33.45.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	1.724	1.749	1.774	1.799	1.824	1.849	1.874
C_p (J K^{-1}mol^{-1})	312.5	317.0	321.5	326.0	330.5	335.1	339.7
c_{sat} (J K^{-1}g^{-1})	1.724	1.749	1.774	1.799	1.824	1.849	1.874
C_{sat} (J K^{-1}mol^{-1})	312.5	317.0	321.5	326.0	330.6	335.1	339.7
Temp. (K)	440	450	460	470	480	490	500
c_p (J K^{-1}g^{-1})	1.900	1.925	1.950	1.976	2.001	2.027	2.052
C_p (J K^{-1}mol^{-1})	344.3	348.9	353.5	358.1	362.7	367.3	371.9
c_{sat} (J K^{-1}g^{-1})	1.900	1.925	1.951	1.976	2.002	2.027	2.052
C_{sat} (J K^{-1}mol^{-1})	344.3	348.9	353.5	358.2	362.8	367.4	372.0
Temp. (K)	510	520	530	540	550	560	570
c_p (J K^{-1}g^{-1})	2.077	2.102	2.127	2.152	2.177	2.202	2.227
C_p (J K^{-1}mol^{-1})	376.5	381.0	385.6	390.1	394.6	399.1	403.6
c_{sat} (J K^{-1}g^{-1})	2.078	2.103	2.128	2.153	2.178	2.202	2.227
C_{sat} (J K^{-1}mol^{-1})	376.6	381.1	385.7	390.2	394.7	399.1	403.6
Temp. (K)	580	590	600	610	620	630	640
c_p (J K^{-1}g^{-1})	2.251	2.275	2.299	2.323	2.347	2.370	2.393
C_p (J K^{-1}mol^{-1})	408.0	412.4	416.7	421.0	425.3	429.5	433.7
c_{sat} (J K^{-1}g^{-1})	2.251	2.275	2.298	2.322	2.345	2.368	2.390
C_{sat} (J K^{-1}mol^{-1})	407.9	412.3	416.6	420.8	425.0	429.1	433.2
Temp. (K)	650	660	670	680	690	700	710
c_p (J K^{-1}g^{-1})	2.415	2.438	2.460	2.481	2.503	2.524	2.544
C_p (J K^{-1}mol^{-1})	437.8	441.8	445.8	449.7	453.6	457.4	461.1
c_{sat} (J K^{-1}g^{-1})	2.412	2.434	2.455	2.476	2.496	2.516	2.535
C_{sat} (J K^{-1}mol^{-1})	437.2	441.1	444.9	448.7	452.4	456.0	459.5
Temp. (K)	720	730	740	750			
c_p (J K^{-1}g^{-1})	2.564	2.584	2.603	2.622			
C_p (J K^{-1}mol^{-1})	464.7	468.3	471.8	475.2			
c_{sat} (J K^{-1}g^{-1})	2.554	2.573	2.590	2.608			
C_{sat} (J K^{-1}mol^{-1})	462.9	466.2	469.5	472.6			

TABLE 33.45.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	28	0.556	1.45–1	0.28	2.86–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
366.1–750.0	890.00	1.72334	1.43924–2	1.70380+1	5.15881+1		III



Name: 2,3,4,9–Tetrahydro–9–methyl–1*H*–carbazole
Formula: $C_{13}H_{15}N$

CAS–RN: 6303–88–4
Group No.: 33–046
Molar Mass: 185.27

TABLE 33.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
92STE/CHI1	330.0–650.0	17	1.00	99.85	melpt	C_{sat}	BDHT	89KNI/ARC
92STE/CHI1	330.0–517.8	17	0.10	99.85	melpt	C_{sat}	BSAO	47HUF

TABLE 33.46.2. Correlated heat capacities sample

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
92STE/CHI1	330.0–650.0	17	1.00	0.081	4.23–2	0.08	4.03–3	3
92STE/CHI1	330.0–517.8	17	0.10#	0.323	1.55–2	0.03	–2.90–5	–1

TABLE 33.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.251	3.39–2	0.07	2.00–3	2
C_{sat}	34	34	0.254	3.66–2	0.07	1.03–3	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
330.0–650.0	1.36318+1	6.21328	4.54743–1	–5.07183–2	II
330.0–650.0	1.39932+1	5.94504	5.20279–1	–5.59895–2	II

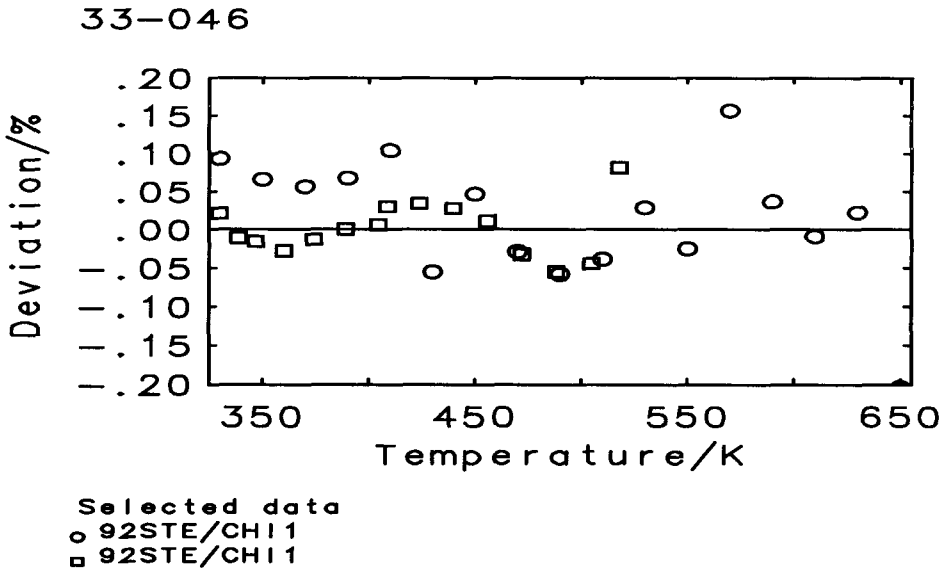
TABLE 33.46.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	1.672	1.706	1.740	1.774	1.808	1.841	1.875
C_p ($J K^{-1} mol^{-1}$)	309.8	316.1	322.4	328.6	334.9	341.1	347.3
c_{sat} ($J K^{-1} g^{-1}$)	1.672	1.706	1.740	1.774	1.808	1.841	1.875
C_{sat} ($J K^{-1} mol^{-1}$)	309.8	316.1	322.4	328.6	334.9	341.1	347.3
Temp. (K)	400	410	420	430	440	450	460
c_p ($J K^{-1} g^{-1}$)	1.908	1.941	1.974	2.007	2.040	2.072	2.105
C_p ($J K^{-1} mol^{-1}$)	353.5	359.6	365.8	371.9	377.9	384.0	389.9
c_{sat} ($J K^{-1} g^{-1}$)	1.908	1.941	1.974	2.007	2.040	2.072	2.105
C_{sat} ($J K^{-1} mol^{-1}$)	353.5	359.6	365.8	371.9	377.9	384.0	389.9
Temp. (K)	470	480	490	500	510	520	530
c_p ($J K^{-1} g^{-1}$)	2.137	2.169	2.200	2.232	2.263	2.294	2.324
C_p ($J K^{-1} mol^{-1}$)	395.9	401.8	407.6	413.5	419.2	424.9	430.6
c_{sat} ($J K^{-1} g^{-1}$)	2.137	2.169	2.200	2.232	2.263	2.293	2.324
C_{sat} ($J K^{-1} mol^{-1}$)	395.9	401.8	407.6	413.5	419.2	424.9	430.5
Temp. (K)	540	550	560	570	580	590	600
c_p ($J K^{-1} g^{-1}$)	2.354	2.384	2.414	2.443	2.471	2.500	2.528
C_p ($J K^{-1} mol^{-1}$)	436.2	441.7	447.2	452.6	457.9	463.1	468.3
c_{sat} ($J K^{-1} g^{-1}$)	2.354	2.384	2.413	2.442	2.471	2.499	2.527
C_{sat} ($J K^{-1} mol^{-1}$)	436.1	441.6	447.1	452.4	457.7	463.0	468.1
Temp. (K)	610	620	630	640	650		
c_p ($J K^{-1} g^{-1}$)	2.555	2.583	2.609	2.636	2.661		
C_p ($J K^{-1} mol^{-1}$)	473.4	478.5	483.4	488.3	493.1		
c_{sat} ($J K^{-1} g^{-1}$)	2.554	2.581	2.607	2.633	2.659		
C_{sat} ($J K^{-1} mol^{-1}$)	473.2	478.2	483.0	487.9	492.6		

TABLE 33.46.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.698	4.36–2	0.10	2.05–2	15

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
330.0–650.0	854.00	8.80270	2.44235–1	1.04536+1	7.93164+1	II


33–046
.20
.15
.10
.05
.00
–.05
–.10
–.15
–.20
Deviation/%
350
450
550
650
Temperature/K
Selected data
92STE/CHI1
92STE/CHI1

34. Miscellaneous Nitrogen Compounds

This family consists of 13 different compounds containing carbon, hydrogen, and nitrogen which do not fit in any of the previous families. All of the compounds except one were measured at several temperatures and each of them was studied only by one laboratory.

Four methyl derivatives of hydrazine were studied between the melting point and room temperature at PSC (51AST/FIN, 51AST/JAN, 53AST/WOO, 55AST/ZOL) with a reported error of 0.2 %. Additional measurements on three higher derivatives of hydrazine (1,1-dimethylhydrazine, 1,2-dimethylhydrazine, and trimethylhydrazine) were carried out in the former Soviet Union at CIUG (81LEB/RYA) using adiabatic calorimetry (76LEB/LIT).

For measurements on cyanamide, carried out at SUU (83DEW/DEK), the initial heating was followed by self-heating of the sample. This compound has explosive and self-reactive properties. The authors recommend 92±2 $J.K^{-1}.mol^{-1}$ for the average value of the heat capacity in the temperature range 324 to 334 K. *Trans*-azobenzene was studied in the same laboratory (84VAN/BOU, 85BOU/DEL) results gave a claimed error of 0.3 to 0.5 %.

Diphenylcarbodiimide and 1,6-diisocyanohexane were studied at CIUG (83BYK/LEB1, 84LEB/BYK1) and the results gave a claimed error of 0.3 %. The data for 3-(dimethylamino)propionitrile presented by (82DZH/KAR1) from ANAZ are given only in graphical form; here, the claimed error of 0.2 % appears unrealistic.

Name: Cyanamide
Formula: CH_2N_2

CAS-RN: 420-04-2
Group No.: 34-001
Molar Mass: 42.04

TABLE 34.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83DEW/DEK	324.4–334.5	4	*nosp*	99.97	*melpt*	C_p	BSAO	79SCH/OFF

TABLE 34.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.593	1.96–1	1.78	5.24–3	0
Temp. range K		A_1					Level of uncertainty
324.4–334.5		1.10480+1					V

TABLE 34.1.4. Recommended values of heat capacities

Temp. (K)	320	330
c_p ($J K^{-1}g^{-1}$)	2.19	2.19
C_p ($J K^{-1}mol^{-1}$)	91.9	91.9

Name: Methylhydrazine
Formula: CH_6N_2

CAS–RN: 60–34–4
Group No.: 34–002
Molar Mass: 46.07

TABLE 34.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51AST/FIN	220.8–298.2	9S	0.20	99.75	melpt	C_p	BSAO	51AST/FIN

TABLE 34.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.113	3.61–3	0.02	1.48–6	–1

Temp. range K	A_1	A_2	Level of uncertainty
220.8–298.2	1.43517+1	6.28031–1	II

TABLE 34.2.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	2.851	2.862	2.873	2.885	2.896	2.900	2.907
C_p ($J\,K^{-1}mol^{-1}$)	131.3	131.9	132.4	132.9	133.4	133.6	133.9

Temp. (K)	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.919	2.928	2.930
C_p ($J\,K^{-1}mol^{-1}$)	134.5	134.9	135.0

TABLE 34.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.109	3.46–3	0.02	1.38–6	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
220.8–298.2	567.00	–4.28028–1	1.68977–2	1.44461+1	2.71054	II

Name: 1,1–Dimethylhydrazine
Formula: $C_2H_8N_2$

CAS–RN: 57–14–7
Group No.: 34–003
Molar Mass: 60.10

TABLE 34.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53AST/WOO	216.0–298.1	18S	0.20	99.99	melpt	C_p	BSAO	47AST/SZA

TABLE 34.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.237	9.12–3	0.05	6.04–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
215.9–298.1		–6.16860	2.54664+1	–9.00779	1.13411		II

TABLE 34.3.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J K^{-1}g^{-1}$)	2.537	2.567	2.593	2.617	2.640	2.663	2.670
C_p ($J K^{-1}mol^{-1}$)	152.5	154.2	155.8	157.3	158.7	160.0	160.5
Temp. (K)	280	290	298.15	300			
c_p ($J K^{-1}g^{-1}$)	2.686	2.710	2.732	2.737			
C_p ($J K^{-1}mol^{-1}$)	161.4	162.9	164.2	164.5			

Name: 1,2–Dimethylhydrazine
Formula: $C_2H_8N_2$

CAS–RN: 540–73–8
Group No.: 34–004
Molar Mass: 60.10

TABLE 34.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51AST/JAN	264.3–298.2	5S	0.20	99.75	melpt	C_p	BSAO	47AST/SZA

TABLE 34.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.135	5.52–3	0.03	1.14–6	0
Temp. range K		A_1	A_2				Level of uncertainty
264.3–298.2		1.80696+1	8.37070–1				III

TABLE 34.4.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	2.813	2.816	2.824	2.836	2.845	2.847
C_p ($J K^{-1}mol^{-1}$)	169.0	169.3	169.7	170.4	171.0	171.1

Name: Trimethylhydrazine
Formula: $C_3H_{10}N_2$

CAS-RN: 1741-01-1
Group No.: 34-005
Molar Mass: 74.13

TABLE 34.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55AST/ZOL	N	205.4–293.9	15	0.20	97.4	melpt	C_p	BSAO	47AST/SZA

55AST/ZOL values were corrected for presence of 1,1-Dimethylhydrazine (2 mol.%)

TABLE 34.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	15	15	0.622	2.77-2	0.12	4.93-5	3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
205.4–293.9	-1.28949+1	3.92118+1	-1.45795+1	1.81061	III

TABLE 34.5.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	2.459	2.477	2.490	2.497	2.502	2.504	2.505
C_p (J K^{-1}mol^{-1})	182.3	183.6	184.6	185.1	185.4	185.6	185.7
Temp. (K)	273.15	280	290	298.15			
c_p (J K^{-1}g^{-1})	2.505	2.506	2.509	2.513			
C_p (J K^{-1}mol^{-1})	185.7	185.8	186.0	186.3			

Name: 3-(Dimethylamino)propanenitrile
Formula: $C_5H_{10}N_2$

CAS-RN: 1738-25-6
Group No.: 34-006
Molar Mass: 98.15

TABLE 34.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82DZH/KAR1	228.0–298.1	9S	0.20	99.18	melpt	C_p	BSAO	54STR/ICK

TABLE 34.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	9	9	0.429	2.14-2	0.09	-1.17-5	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
228.0–298.1	1.38949+2	-1.35798+2	5.28543+1	-6.72978	V

TABLE 34.6.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.06	2.07	2.09	2.11	2.13	2.14	2.15
C_p (J K^{-1}mol^{-1})	202	203	205	207	209	210	211
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	2.16	2.16	2.16				
C_p (J K^{-1}mol^{-1})	212	212	212				

Name: Phenylhydrazine
Formula: $C_6H_8N_2$

CAS-RN: 100-63-0
Group No.: 34-007
Molar Mass: 108.14

TABLE 34.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEB/RYA		293.2–357.8	5	0.30	99.8	melpt	C_p	BSAO	76LEB/LIT
81LEB/RYA	N	335.5–385.5	3	1.00	99.8	melpt	C_{avg}	DSIO	76LEB/RYA

81LEB/RYA average values in temperature ranges 298–373 K, 298–423 K and 298–473 K

TABLE 34.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	5	1.029	8.20–2	0.31	2.88–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
293.2–357.8		1.81909+1	2.63109				III

TABLE 34.7.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1}g^{-1}$)	2.005	2.026	2.046	2.066	2.086	2.107	2.127
C_p ($J K^{-1}mol^{-1}$)	216.9	219.1	221.3	223.4	225.6	227.8	230.0
Temp. (K)	370	380	390	400			
c_p ($J K^{-1}g^{-1}$)	2.147	2.167	2.188	2.208			
C_p ($J K^{-1}mol^{-1}$)	232.2	234.4	236.6	238.8			

Name: (1-Methylethylidene)hydrazone 2-propanone
Formula: $C_6H_{12}N_2$

CAS-RN: 627-70-3
Group No.: 34-008
Molar Mass: 112.17

TABLE 34.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEB/RYA	308.1–344.7	5	0.30	99.8	melpt	C_p	BSAO	76LEB/LIT

TABLE 34.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.326	1.92–2	0.10	2.21–5	1
Temp. range K		A_1	A_2				Level of uncertainty
308.1–344.7		1.58436+1	1.18077				III

TABLE 34.8.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.446	1.454	1.463	1.472
C_p ($J K^{-1} mol^{-1}$)	162.2	163.1	164.1	165.1

Name: Phenylhydrazone acetaldehyde
Formula: $C_8H_{10}N_2$

CAS–RN: 935–07–9
Group No.: 34–009
Molar Mass: 134.18

TABLE 34.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEB/RYA	301.2–328.2	5	0.30	99.5	melpt	C_p	DSIO	76LEB/RYA

TABLE 34.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.888	9.19–2	0.27	5.98–4	1

Temp. range K	A_1	A_2	Level of uncertainty
301.2–328.2	–6.20525+1	2.98155+1	III

TABLE 34.9.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.697	1.882	2.067	2.252
C_p ($J K^{-1} mol^{-1}$)	227.8	252.6	277.3	302.1

Name: 1,6–Diisocyanohexane
Formula: $C_8H_{12}N_2$

CAS–RN: 929–57–7
Group No.: 34–010
Molar Mass: 136.20

TABLE 34.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83BYK/LEB1	206.1–330.0	4S	0.30	99.53	melpt	C_p	BSAO	76LEB/LIT

TABLE 34.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.380	3.98–2	0.11	2.10–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
206.1–330.0		3.03267+1	1.73045–1	5.04881–1			III

TABLE 34.10.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	2.009	2.024	2.039	2.054	2.070	2.087	2.105
C_p (J K^{-1}mol^{-1})	273.7	275.6	277.7	279.8	282.0	284.3	286.6
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.110	2.123	2.141	2.157	2.160	2.180	2.201
C_p (J K^{-1}mol^{-1})	287.4	289.1	291.6	293.8	294.2	297.0	299.7
Temp. (K)	330						
c_p (J K^{-1}g^{-1})	2.222						
C_p (J K^{-1}mol^{-1})	302.6						

Name: Diphenyldiazene
Formula: $C_{12}H_{10}N_2$

CAS–RN: 103–33–3
Group No.: 34–011
Molar Mass: 182.22

TABLE 34.11.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
08BOG/WIN	N	356.65	1.724	nosp	not specified		C_{avg}	DSIO	08BOG/WIN

08BOG/WIN average value in temperature range 341–372 K

Name: (*E*)–Diphenyldiazene
Formula: $C_{12}H_{10}N_2$

CAS–RN: 17082–12–1
Group No.: 34–012
Molar Mass: 182.22

TABLE 34.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
84VAN/BOU	344.6–356.2	4	nosp	99.87	melpt	C_p	BSAO	79SCH/OFF
85BOU/DEL	343.6–408.4	27	nosp	99.84	melpt	C_p	BSAO	85BOU/DEL

TABLE 34.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
85BOU/DEL	343.6–408.4	27	0.40#	0.108	1.64-2	0.04	1.30–5	0
				Rejected data				
84VAN/BOU	(1.69–1, 0.46, –1.68–1, –4)							

TABLE 34.12.3. Parameters of regression polynomial

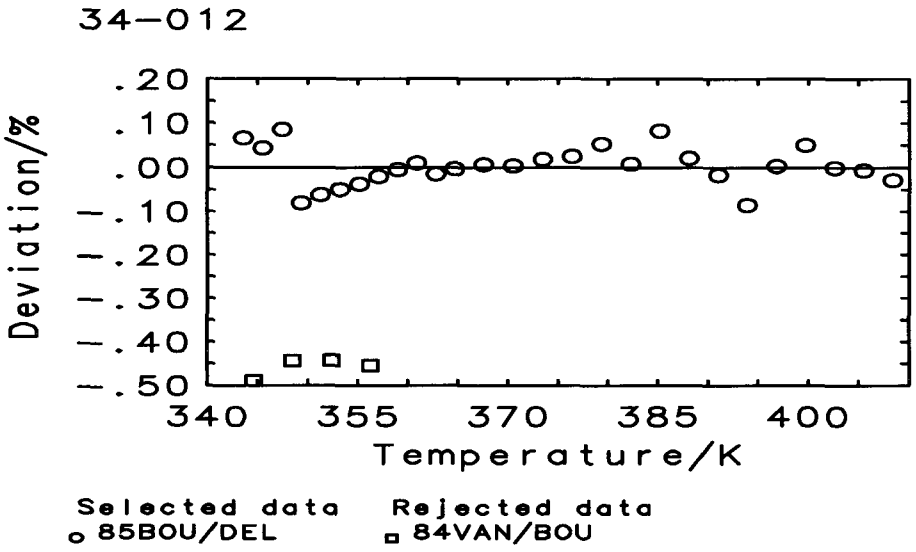
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	27	0.113	1.70–2	0.05	1.30–5	0
Temp. range K		A_1	A_2				Level of uncertainty
343.6–408.4		1.58572+1	5.96832				III

TABLE 34.12.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1} g^{-1}$)	1.677	1.704	1.731	1.758	1.786	1.813	1.840
C_p ($J K^{-1} mol^{-1}$)	305.5	310.5	315.5	320.4	325.4	330.3	335.3

TABLE 34.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	31	0.441	5.60–2	0.15	2.84–3	1 2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
343.6–408.4	807.00	2.43031+1	1.66392	9.08184	8.87423+1		III



Name: *N,N'*–Methanetetraylbisbenzenamine
Formula: $C_{13}H_{10}N_2$

CAS–RN: 622–16–2
Group No.: 34–013
Molar Mass: 194.24

TABLE 34.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84LEB/BYK1	287.4–330.0	3S	0.30	99.7	melpt	C_p	BSAO	76LEB/LIT

TABLE 34.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.138	1.51–2	0.04	2.54–6	0
Temp. range K		A_1	A_2				Level of uncertainty
287.4–330.0		2.11683+1	5.18346				III

TABLE 34.13.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.550	1.568	1.572	1.594	1.616	1.638
C_p ($J\,K^{-1}mol^{-1}$)	301.0	304.5	305.3	309.6	313.9	318.2

4. Compounds of Carbon, Hydrogen and Oxygen

41. Ethers

The ether family contains 48 compounds, 19 of which were measured at one temperature only. The data for two compounds have been taken over without any further specification regarding the origin of values from the monograph Glycols (52CUR).

The only laboratory which was paying systematic attention to the heat capacities of ethers was NPLT, where 9 dialkyl ethers of high purity were measured with excellent accuracy between the melting point temperature and an upper temperature typically between 300 and 350 K (71COU/LEE, 74AND/COU, 75AND/COU, 75AND/MAR). In all cases, a high statistical weight has been given to these data in all correlations.

The data on several alkyl phenyl ethers determined at the end of 19th century (*87SCH) were used in the correlation because no other sources of data are available. These data have an estimated error of about 3 %.

For most ethers only one data source was available with the exception of diethyl ether and also diphenyl ether, which is used as a secondary calorimetric standard (53GIN/FUR). In order to develop the recommended values for diethyl ether, we have combined the NPLT data up to 300 K (71COU/LEE) with the values generated at higher temperatures up to 460 K from the equation given by Wilhoit et al. (85WIL/CHA). This equation was based on the data from enthalpy measurements (62EUB/SMI) and two other sources (*62REG, *67HIR). This case is one of the exceptions where we founded our recommendations partly on a secondary source as it seemed to be the best choice. For conversion between C_{sat} and C_p, data were used from the literature (83MCG and 91CDA). Regarding diphenyl ether, we based our recommendations exclusively on the measurements from NBSW (51FUR/GIN) which were available only as smoothed data in the temperature range from 300 to 570 K.

Beside the precise measurements mentioned in the preceding paragraph, reliable data are also available for dimethyl ether from PSC (41KEN/SEG) and for dimethoxymethane from RUH (64MCE/KIL). Studies were carried out for 2,5,8-trioxanonane and 2,5,8,11-tetraoxadodecane at UME (66BEA/CLE) over a temperature range of about 140 K. Results of lower accuracy were obtained for 2,5,8,11,14-pentaoxapentadecane (65KRI/LOE). This ether has a potential for use as a component in cooling agents. Several other ethers were measured over a narrow temperature interval at BTIM (86BER/GUR, 88BAG/GUR) and at USC (78ROU/PER).

Name: Oxybismethane
Formula: C_2H_6O

CAS-RN: 115-10-6
Group No.: 41-001
Molar Mass: 46.07

TABLE 41.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41KEN/SAG	137.2–245.5	31	nosp	100.00	melpt	C_p	BSIO	36AST/MES

TABLE 41.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	31	0.861	3.10–2	0.26	1.40–4	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
137.2–245.5		8.27280	6.42960	–3.92091	8.08992–1		III

TABLE 41.1.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p ($J K^{-1}g^{-1}$)	2.131	2.134	2.136	2.138	2.141	2.145	2.151
C_p ($J K^{-1}mol^{-1}$)	98.19	98.32	98.41	98.50	98.61	98.81	99.11
Temp. (K)	210	220	230	240	250		
c_p ($J K^{-1}g^{-1}$)	2.161	2.176	2.195	2.220	2.253		
C_p ($J K^{-1}mol^{-1}$)	99.57	100.2	101.1	102.3	103.8		

TABLE 41.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	31	0.845	3.04–2	0.25	1.39–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
137.2–245.5	400.00	1.65248+1	5.76202	5.92913	1.18479+1		III

Name: Dimethoxymethane
Formula: $C_3H_8O_2$

CAS–RN: 109–87–5
Group No.: 41–002
Molar Mass: 76.10

TABLE 41.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		295.7–300.9	3S	nosp	not specified		C_{avg}	DSIO	*81VON
64MCE/KIL	N	171.1–307.8	31	nosp	99.9	chrom	C_p	BSIO	55TAY/JOH

64MCE/KIL error below and above 250 K 0.03 % and 0.3 %, respectively

TABLE 41.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	295.7–300.9	3	2.00#	0.124	4.83–2	0.25	1.30–2	1
64MCE/KIL	171.1–307.8	31	0.40#	0.235	1.69–2	0.09	–1.70–5	3

TABLE 41.2.3. Parameters of regression polynomial

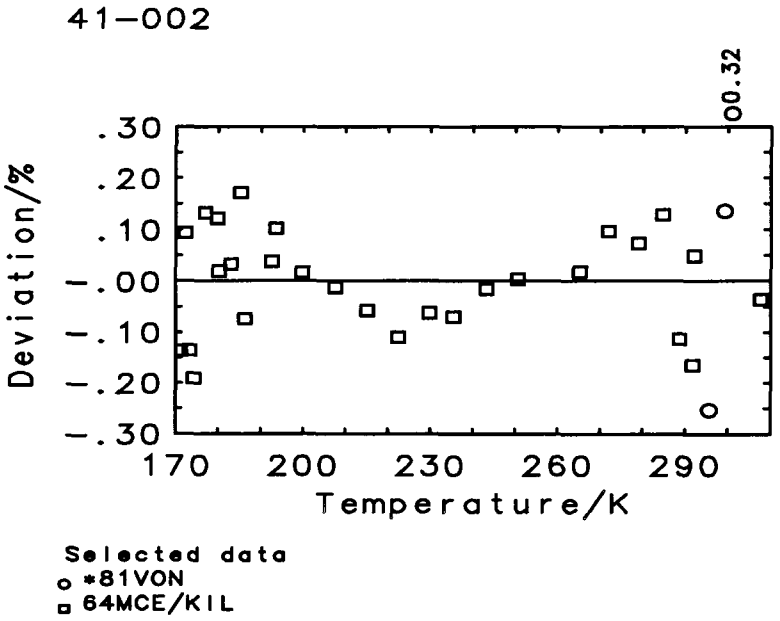
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.242	2.30–2	0.12	1.13–3	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
171.1–307.8		2.05251+1	–4.50681	1.78601	–1.34256–1		II

TABLE 41.2.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.897	1.903	1.911	1.921	1.933	1.948	1.964
C_p (J K^{-1}mol^{-1})	144.4	144.8	145.4	146.2	147.1	148.2	149.4
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.982	2.002	2.024	2.047	2.055	2.072	2.098
C_p (J K^{-1}mol^{-1})	150.8	152.3	154.0	155.8	156.3	157.7	159.7
Temp. (K)	298.15	300	310				
c_p (J K^{-1}g^{-1})	2.120	2.126	2.154				
C_p (J K^{-1}mol^{-1})	161.4	161.7	163.9				

TABLE 41.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.445	3.46–2	0.19	2.64–3	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
171.1–307.8	480.60	1.41954	2.58880	1.38575+1	1.94596–1		II



Name: 2–Methoxy–1–propene
Formula: C_4H_8O

CAS–RN: 116–11–0
Group No.: 41–003
Molar Mass: 72.11

TABLE 41.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BAG/GUR	273.0–301.5	4	2.00	not specified		C_p	BDHT	86CDA/COM

TABLE 41.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.140	5.34–2	0.28	1.52–4	0
Temp. range K		A_1	A_2				Level of uncertainty
273.0–301.5		9.97113	3.16927				V

TABLE 41.3.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.14	2.15	2.17	2.21	2.24	2.25
C_p ($J\,K^{-1}mol^{-1}$)	154	155	157	159	161	162

Name: 1–Methoxypropane
Formula: $C_4H_{10}O$

CAS–RN: 557–17–5
Group No.: 41–004
Molar Mass: 74.12

TABLE 41.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75AND/MAR	137.5–308.9	116	nosp	99.99	melpt	C_p	BSAO	63AND/COU1

TABLE 41.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	116	116	0.210	7.61–3	0.04	6.74–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
137.5–308.9		1.66573+1	–2.23132–1	2.19682–1	7.36744–2		II

TABLE 41.4.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p ($J\,K^{-1}g^{-1}$)	1.904	1.914	1.925	1.938	1.951	1.967	1.983
C_p ($J\,K^{-1}mol^{-1}$)	141.2	141.9	142.7	143.6	144.6	145.8	147.0
Temp. (K)	210	220	230	240	250	260	270
c_p ($J\,K^{-1}g^{-1}$)	2.001	2.021	2.042	2.065	2.089	2.115	2.143
C_p ($J\,K^{-1}mol^{-1}$)	148.3	149.8	151.3	153.0	154.8	156.8	158.9
Temp. (K)	273.15	280	290	298.15	300	310	
c_p ($J\,K^{-1}g^{-1}$)	2.152	2.173	2.205	2.232	2.238	2.274	
C_p ($J\,K^{-1}mol^{-1}$)	159.5	161.1	163.4	165.4	165.9	168.5	

TABLE 41.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	116	116	0.576	2.13–2	0.12	4.32–5	–43
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
137.5–308.9	476.25	–3.73373–1	2.17396	1.37337+1	1.60315–2		II

Name: 2–Methoxypropane
Formula: $C_4H_{10}O$

CAS–RN: 598–53–8
Group No.: 41–005
Molar Mass: 74.12

TABLE 41.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75AND/MAR	130.2–311.4	62	nosp	99.90	melpt	C_p	BSAO	63AND/COU1

TABLE 41.5.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	62	62	0.506	1.78–2	0.10	3.27–5	–9
C_{sat}	62	62	0.515	1.81–2	0.10	3.41–5	–10

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
130.2–220.0	1.96312+1	–5.63095	2.80412	–3.19802–1	II
220.0–311.4	1.56382+1	–1.85978–1	3.29122–1	5.51970–2	II
130.2–220.0	1.96029+1	–5.58023	2.77429	–3.14059–1	II
220.0–311.4	1.62570+1	–1.01759	7.00367–1	1.71964–4	II

TABLE 41.5.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_p (J K^{-1}g^{-1})	1.834	1.836	1.841	1.850	1.861	1.875	1.891
C_p (J K^{-1}mol^{-1})	135.9	136.1	136.5	137.1	137.9	139.0	140.2
c_{sat} (J K^{-1}g^{-1})	1.834	1.836	1.841	1.850	1.861	1.875	1.891
C_{sat} (J K^{-1}mol^{-1})	135.9	136.1	136.5	137.1	137.9	139.0	140.2
Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.910	1.931	1.953	1.977	2.002	2.030	2.058
C_p (J K^{-1}mol^{-1})	141.6	143.1	144.8	146.5	148.4	150.4	152.6
c_{sat} (J K^{-1}g^{-1})	1.910	1.931	1.953	1.977	2.002	2.030	2.058
C_{sat} (J K^{-1}mol^{-1})	141.6	143.1	144.8	146.5	148.4	150.4	152.6
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.089	2.099	2.121	2.155	2.184	2.191	2.229
C_p (J K^{-1}mol^{-1})	154.8	155.6	157.2	159.7	161.9	162.4	165.2
c_{sat} (J K^{-1}g^{-1})	2.088	2.098	2.120	2.154	2.182	2.189	2.225
C_{sat} (J K^{-1}mol^{-1})	154.8	155.5	157.2	159.6	161.7	162.2	164.9

TABLE 41.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	62	0.717	2.53–2	0.14	6.63–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
130.2–311.4	464.48	4.62118+1	3.01342	1.30890+1	4.56982+1	2.03703	5.76902+1	II

Name: 1,1'–Oxybisethane
Formula: $C_4H_{10}O$

CAS–RN: 60–29–7
Group No.: 41–006
Molar Mass: 74.12

TABLE 41.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
07BAT	N	181.8–251.8	5	nosp	not specified		C_p	BSIO	07BAT
24KEY/BEA		274.4–286.5	2	1.00	not specified		C_p	BSIO	24KEY/BEA
26PAR/HUF		164.4–290.0	10	nosp	not specified		C_p	BSIO	25PAR
35AOY/KAN		159.3–255.2	7	nosp	not specified		C_p	BSAO	35AOY/KAN
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
39MAZ2	N	161.3–293.7	72	nosp	not specified		C_p	BSIO	39MAZ3
39MAZ2	N	161.9–293.3	71	nosp	not specified		C_p	BSIO	39MAZ3
39MAZ3	N	164.1–291.1	14	nosp	not specified		C_p	BSIO	39MAZ3
71COU/LEE		159.9–299.4	46	nosp	99.92	melpt	C_p	BSAO	63AND/COU1
85WIL/CHA	N	300.0–460.0	eqn	nosp	not specified		C_p	not specified	

07BAT same data in 08BAT
36KUR/VOS average value in temperature range 290–333 K
39MAZ2 first sample
39MAZ2 second sample
39MAZ3 data from a graph only
85WIL/CHA parameters calculated from enthalpy equation obtained from data by *62REG, *67HIR and 62EUB/SMI

TABLE 41.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71COU/LEE	159.9–299.4	46	0.20#	0.303	1.19–2	0.06	–7.62–4	1
85WIL/CHA	300.0–460.0	33	4.00#	0.956	9.93–1	3.82	5.02–1	13
				Rejected data				
07BAT	(4.83–1, 2.52, 2.87–1, 1)			24KEY/BEA	(1.05, 4.94, 1.05, 2)			
26PAR/HUF	(8.40–2, 0.44,–1.37–3, 0)			35AOY/KAN	(1.38–1, 0.73, 1.32–1, 6)			
36KUR/VOS	(1.05, 5.20,–1.05, –1)			39MAZ2	(7.65–2, 0.39, 2.55–2, 18)			
39MAZ2	(7.68–2, 0.39, 2.55–2, 18)			39MAZ3	(8.38–2, 0.43, 1.65–2, 0)			

TABLE 41.6.3. Parameters of cubic spline polynomials

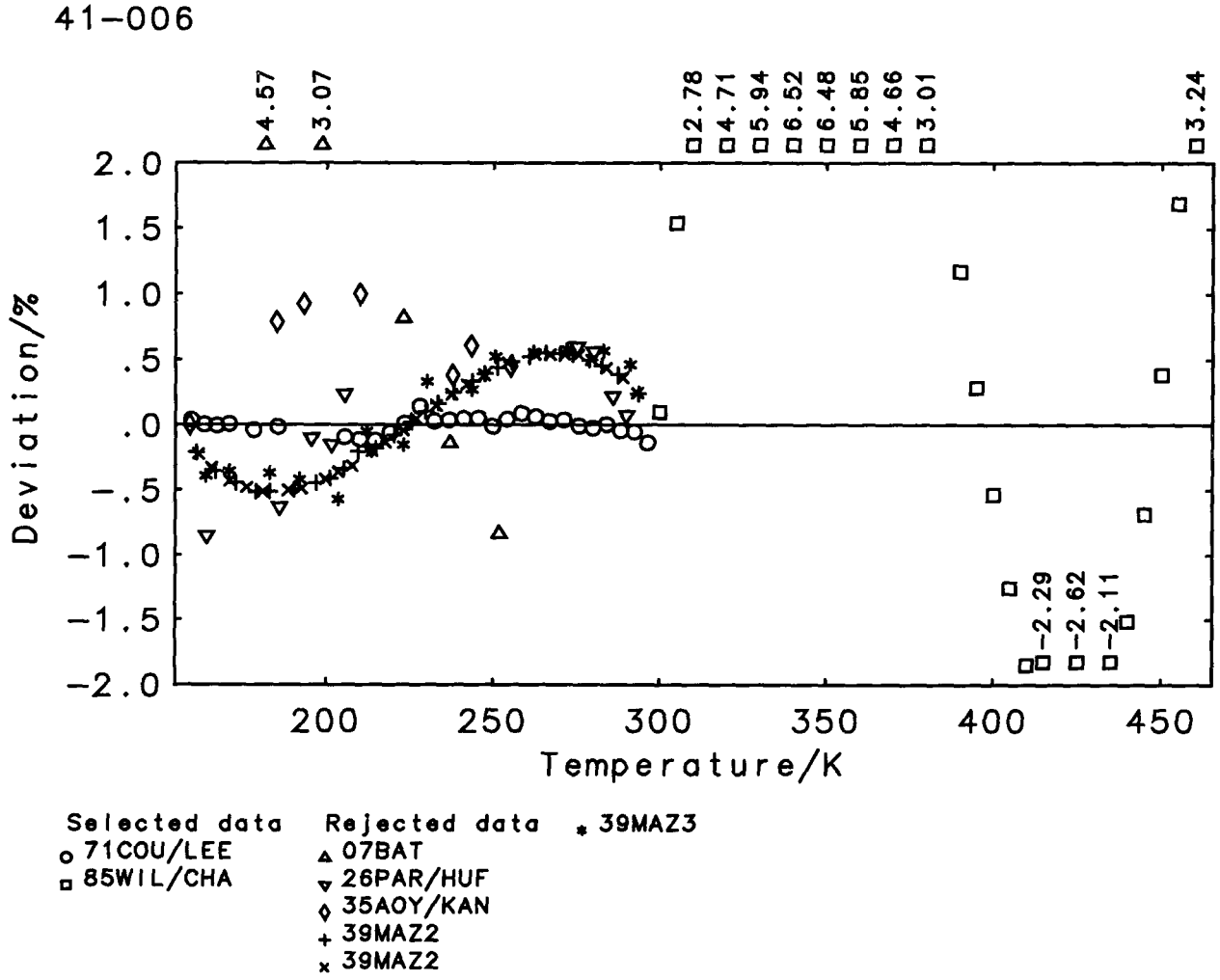
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	261	79	0.686	6.68–1	2.57	2.09–1	14
C_{sat}	261	77	0.665	6.25–1	2.49	2.00–1	16
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
159.9–300.0		7.02243	1.23736+1	–4.63082	6.79719–1		II
300.0–370.0		–1.11357+2	1.30753+2	–4.40907+1	5.06415		VI
370.0–440.0		6.12164+2	–4.55886+2	1.14460+2	–9.21974		VI
159.9–300.0		7.49444	1.16947+1	–4.31108	6.30328–1		II
300.0–370.0		–1.19550+2	1.38739+2	–4.66593+1	5.33569		VI
370.0–440.0		1.06240+3	–8.19595+2	2.12350+2	–1.79985+1		VI

TABLE 41.6.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.991	2.021	2.048	2.073	2.096	2.118	2.139
C_p (J K^{-1}mol^{-1})	147.6	149.8	151.8	153.6	155.3	157.0	158.5
c_{sat} (J K^{-1}g^{-1})	1.991	2.021	2.047	2.072	2.096	2.118	2.139
C_{sat} (J K^{-1}mol^{-1})	147.6	149.8	151.8	153.6	155.3	157.0	158.5
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.160	2.181	2.202	2.225	2.249	2.257	2.275
C_p (J K^{-1}mol^{-1})	160.1	161.6	163.2	164.9	166.7	167.3	168.7
c_{sat} (J K^{-1}g^{-1})	2.160	2.181	2.203	2.225	2.249	2.257	2.275
C_{sat} (J K^{-1}mol^{-1})	160.1	161.7	163.3	164.9	166.7	167.3	168.6
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.304	2.329	2.335	2.37	2.41	2.46	2.53
C_p (J K^{-1}mol^{-1})	170.8	172.6	173.1	176	179	183	188
c_{sat} (J K^{-1}g^{-1})	2.302	2.327	2.333	2.37	2.41	2.46	2.52
C_{sat} (J K^{-1}mol^{-1})	170.7	172.5	172.9	175	178	182	187
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.61	2.72	2.84	3.00	3.17	3.36	3.55
C_p (J K^{-1}mol^{-1})	194	201	211	222	235	249	263
c_{sat} (J K^{-1}g^{-1})	2.61	2.71	2.84	2.99	3.16	3.33	3.50
C_{sat} (J K^{-1}mol^{-1})	193	201	210	222	234	247	259
Temp. (K)	420	430	440				
c_p (J K^{-1}g^{-1})	3.75	3.95	4.13				
C_p (J K^{-1}mol^{-1})	278	293	306				
c_{sat} (J K^{-1}g^{-1})	3.64	3.76	3.82				
C_{sat} (J K^{-1}mol^{-1})	270	278	283				

TABLE 41.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	261	79	2.331	2.67	8.34	1.15	28
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
159.9–460.0	466.74	–2.18920	3.31924–1	1.49270+1	4.49789	–3.59265–1	1.00097–2	V



Name: 1,2–Dimethoxyethane
Formula: $C_4H_{10}O_2$

CAS–RN: 110–71–4
Group No.: 41–007
Molar Mass: 90.12

TABLE 41.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KUS/SUU	298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 41.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KUS/SUU	298.1	1	0.10	0.000	0.00	0.00	0.00	0
				Rejected data				
91TRE/COS	(2.60–1, 1.13,–2.60–1, –1)							

TABLE 41.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		2.32485+1					III

TABLE 41.7.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.145
C_p (J K^{-1}mol^{-1})	193.3

Name: 1-Ethoxypropane
Formula: $C_5H_{12}O$

CAS-RN: 628-32-0
Group No.: 41-008
Molar Mass: 88.15

TABLE 41.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75AND/MAR	151.3–316.3	62	nosp	99.98	melpt	C_p	BSAO	63AND/COU1

TABLE 41.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	62	0.294	1.37–2	0.06	1.45–5	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
151.3–316.3		1.22757+1	8.99674	–3.24807	5.09163–1		II

TABLE 41.8.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.904	1.928	1.951	1.973	1.994	2.014	2.034
C_p (J K^{-1}mol^{-1})	167.8	170.0	172.0	173.9	175.7	177.5	179.3
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	2.053	2.073	2.094	2.115	2.137	2.161	2.169
C_p (J K^{-1}mol^{-1})	181.0	182.8	184.6	186.4	188.4	190.5	191.2
Temp. (K)	280	290	298.15	300	310	320	
c_p (J K^{-1}g^{-1})	2.186	2.214	2.237	2.243	2.275	2.310	
C_p (J K^{-1}mol^{-1})	192.7	195.1	197.2	197.7	200.5	203.6	

TABLE 41.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	62	62	0.864	3.82–2	0.17	1.24–4	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
151.3–316.3	500.23	–2.81004	4.00582–1	1.72369+1	4.92804		II

Name: 1–Methoxybutane
Formula: $C_5H_{12}O$

CAS–RN: 628–28–4
Group No.: 41–009
Molar Mass: 88.15

TABLE 41.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75AND/MAR	160.2–315.7	52	nosp	99.98	melpt	C_p	BSAO	63AND/COU1
82VIL/CAS	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 41.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75AND/MAR	160.2–315.7	52	0.20#	0.238	1.04–2	0.05	1.05–5	–2
				Rejected data				
82VIL/CAS	(3.97–2, 0.17,–3.97–2, –1)							

TABLE 41.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	52	0.246	1.07–2	0.05	1.05–5	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
160.2–315.7		2.13507+1	–2.02096	8.83884–1			II

TABLE 41.9.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.922	1.931	1.941	1.953	1.966	1.981	1.998
C_p (J K^{-1}mol^{-1})	169.4	170.2	171.1	172.1	173.3	174.6	176.1
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.016	2.037	2.058	2.082	2.107	2.115	2.134
C_p (J K^{-1}mol^{-1})	177.7	179.5	181.4	183.5	185.7	186.5	188.1
Temp. (K)	290	298.15	300	310	320		
c_p (J K^{-1}g^{-1})	2.162	2.187	2.192	2.224	2.258		
C_p (J K^{-1}mol^{-1})	190.6	192.8	193.3	196.1	199.0		

TABLE 41.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	52	0.586	2.58–2	0.12	5.20–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
160.2–315.7	502.00	7.02598–1	3.20510	1.58896+1	3.85046–2		II

Name: 2–Methoxy–2–methylpropane
Formula: $C_5H_{12}O$

CAS–RN: 1634–04–4
Group No.: 41–010
Molar Mass: 88.15

TABLE 41.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36EVA/EDL	298.1	1	nosp	not specified		C_p	not specified	
75AND/MAR	168.3–308.4	38	nosp	99.95	melpt	C_p	BSAO	63AND/COU1

TABLE 41.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75AND/MAR	168.3–308.4	38	0.20#	0.380	1.50–2	0.08	2.17–5	3
				Rejected data				
36EVA/EDL	(7.14–2, 0.32, 7.14–2, 1)							

TABLE 41.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	38	0.396	1.56–2	0.08	2.17–5	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
168.3–308.4		1.70936+1	–2.99989–1	7.14585–1			II

TABLE 41.10.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.759	1.780	1.802	1.825	1.850	1.876	1.904
C_p (J K^{-1}mol^{-1})	155.1	156.9	158.8	160.9	163.1	165.4	167.8
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.933	1.963	1.994	2.027	2.038	2.062	2.097
C_p (J K^{-1}mol^{-1})	170.4	173.0	175.8	178.7	179.6	181.7	184.9
Temp. (K)	298.15	300	310				
c_p (J K^{-1}g^{-1})	2.127	2.134	2.172				
C_p (J K^{-1}mol^{-1})	187.5	188.1	191.5				

TABLE 41.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	38	0.562	2.30–2	0.11	4.64–5	5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
168.3–308.4	497.10	–3.80219	1.39538	1.40341+1	2.59010	II

Name: 2,2–Dimethoxypropane
Formula: $C_5H_{12}O_2$

CAS–RN: 77–76–9
Group No.: 41–011
Molar Mass: 104.15

TABLE 41.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86BER/GUR	N	273.0–334.1	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 84BAG/BAE and 88BAG/GUR

TABLE 41.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.499	2.69–1	01.00	2.87–3	2

Temp. range K	A_1	A_2	Level of uncertainty
273.0–334.1	1.24878+1	4.59914	V

TABLE 41.11.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.99	2.00	2.02	2.06	2.09	2.10	2.14
C_p (J K^{-1}mol^{-1})	207	208	211	215	218	219	222

Temp. (K)	320	330
c_p (J K^{-1}g^{-1})	2.17	2.21
C_p (J K^{-1}mol^{-1})	226	230

Name: 1–Ethoxy–2–methoxyethane
Formula: $C_5H_{12}O_2$

CAS–RN: 5137–45–1
Group No.: 41–012
Molar Mass: 104.15

TABLE 41.12.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73KUS/SUU	298.15	2.157	0.10	not specified		C_p	DDCT	71KON/SUU

Name: 1–(Ethenyloxy)butane
Formula: $C_6H_{12}O$

CAS–RN: 111–34–2
Group No.: 41–013
Molar Mass: 100.16

TABLE 41.13.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47SCH/ZOS	298.15	2.314	nosp	not specified		C_p	not specified	

Name: 1–(Ethenyloxy)–2–methylpropane
Formula: $C_6H_{12}O$

CAS–RN: 109–53–5
Group No.: 41–014
Molar Mass: 100.16

TABLE 41.14.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47SCH/ZOS	298.15	2.322	nosp	not specified		C_p	not specified	

Name: 2–Ethoxy–2–methylpropane
Formula: $C_6H_{14}O$

CAS–RN: 637–92–3
Group No.: 41–015
Molar Mass: 102.18

TABLE 41.15.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36EVA/EDL	298.15	2.134	nosp	not specified		C_p	not specified	

Name: 2–Methoxy–2–methylbutane
Formula: $C_6H_{14}O$

CAS–RN: 994–05–8
Group No.: 41–016
Molar Mass: 102.18

TABLE 41.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36EVA/EDL	298.1	1	nosp	not specified		C_p	not specified	
91ROZ/SAF	298.1	1	nosp	99.6	chrom	C_p	BDHT	69PER/COM

TABLE 41.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
91ROZ/SAF	298.1	1	3.00#	0.000	0.00	0.00	0.00	0
				Rejected data				
36EVA/EDL	(6.84, 25.59, 6.84, 1)							

TABLE 41.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		1.98958+1					V

TABLE 41.16.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1} g^{-1}$)	1.62
C_p ($J K^{-1} mol^{-1}$)	165

Name: 1,1'–Oxybispropane
Formula: $C_6H_{14}O$

CAS–RN: 111–43–3
Group No.: 41–017
Molar Mass: 102.18

TABLE 41.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75AND/COU	160.6–322.7	66	nosp	99.97	melpt	C_p	BSAO	63AND/COU1
83KIM/TRE	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED

TABLE 41.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75AND/COU	160.6–322.7	66	0.20#	0.232	1.22–2	0.05	4.99–5	–3
83KIM/TRE	298.1	1	0.50#	0.119	1.58–2	0.06	–1.58–2	–1

TABLE 41.17.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	67	67	0.240	1.27–2	0.05	–1.87–4	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
160.6–240.0		1.68819+1	7.02346	–2.79567	5.19798–1		II
240.0–322.7		2.37149+1	–1.51776	7.63170–1	2.55141–2		II

TABLE 41.17.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J K^{-1}g^{-1}$)	1.879	1.896	1.912	1.929	1.945	1.962	1.980
C_p ($J K^{-1}mol^{-1}$)	192.0	193.7	195.4	197.0	198.8	200.5	202.4
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.999	2.020	2.042	2.065	2.090	2.098	2.116
C_p ($J K^{-1}mol^{-1}$)	204.3	206.4	208.6	211.0	213.5	214.4	216.2
Temp. (K)	290	298.15	300	310	320		
c_p ($J K^{-1}g^{-1}$)	2.145	2.169	2.174	2.206	2.239		
C_p ($J K^{-1}mol^{-1}$)	219.1	221.6	222.2	225.4	228.7		

TABLE 41.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	67	67	0.309	1.60–2	0.06	–7.04–4	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
160.6–322.7	530.60	–2.50300	2.58455	1.83362+1	6.06005–1		II

Name: 2,2'–Oxybispropane
Formula: $C_6H_{14}O$

CAS–RN: 108–20–3
Group No.: 41–018
Molar Mass: 102.18

TABLE 41.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33PAR/HUF		194.5–293.1	8	1.00	not specified		C_p	BSIO	25PAR
61ROU	N	296.1–318.1	2	nosp	not specified		C_p	BSAO	61ROU
74AND/COU		187.8–340.0	19S	nosp	99.86	melpt	C_p	BSAO	63AND/COU1
91GRO/ROU		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

61ROU constant value in temperature range 296–318 K obtained by the author

TABLE 41.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74AND/COU	187.8–340.0	19	0.20#	0.121	5.59–3	0.02	2.51–6	0
				Rejected data				
33PAR/HUF	(2.16–1, 0.88, 2.07–1, 8)			61ROU	(6.09–1, 2.33,–3.21–1, 0)			
91GRO/ROU	(6.61–2, 0.25, 6.61–2, 1)							

TABLE 41.18.3. Parameters of regression polynomial

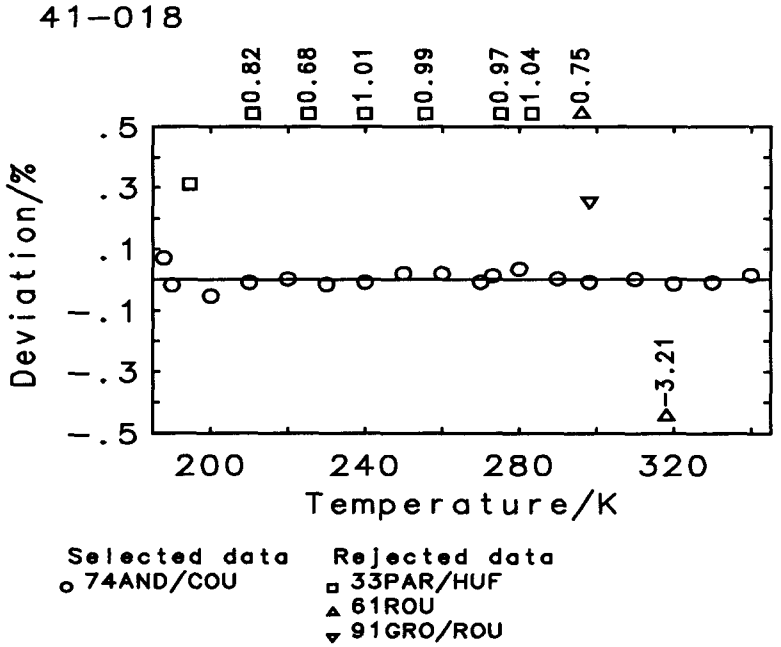
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	30	19	0.132	6.09–3	0.03	2.51–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
187.8–340.0		2.07935+1	–1.04875	9.36687–1			II

TABLE 41.18.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.805	1.826	1.849	1.873	1.899	1.926	1.955
C_p (J K^{-1}mol^{-1})	184.4	186.6	188.9	191.4	194.0	196.8	199.8
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.985	2.017	2.028	2.051	2.086	2.115	2.122
C_p (J K^{-1}mol^{-1})	202.9	206.1	207.2	209.5	213.1	216.1	216.8
Temp. (K)	310	320	330	340			
c_p (J K^{-1}g^{-1})	2.160	2.199	2.240	2.283			
C_p (J K^{-1}mol^{-1})	220.7	224.7	228.9	233.3			

TABLE 41.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	30	19	0.637	3.11–2	0.13	6.42–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
187.8–340.0	500.32	–4.41547	1.23510	1.65528+1	3.94633		II



Name: 1,1–Diethoxyethane
Formula: $C_6H_{14}O_2$

CAS–RN: 105–57–7
Group No.: 41–019
Molar Mass: 118.18

TABLE 41.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		316.7–338.5	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*98LOU	N	332.2	1	nosp	not specified		C_{avg}	DSIO	*98LOU

*98LOU average value in temperature range 292–372 K

TABLE 41.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	316.7–338.5	4	2.00#	0.086	5.25–2	0.17	–5.10–2	–4
*98LOU	332.2	1	3.00#	0.512	4.75–1	1.54	4.75–1	1

TABLE 41.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.312	2.81–1	0.91	5.42–2	–3

Temp. range K	A_1	A_2	Level of uncertainty
316.7–338.5	1.03712+1	6.04007	V

TABLE 41.19.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J\,K^{-1}g^{-1}$)	2.09	2.13	2.17
C ($J\,K^{-1}mol^{-1}$)	247	252	257

Name: 1,2–Diethoxyethane
Formula: $C_6H_{14}O_2$

CAS–RN: 629–14–1
Group No.: 41–020
Molar Mass: 118.18

TABLE 41.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KUS/SUU	298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
82VIL/CAS	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
84BEN/KUM	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 41.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KUS/SUU	298.1	1	0.10	1.155	3.60–2	0.12	–3.60–2	–1
82VIL/CAS	298.1	1	0.30	1.762	1.66–1	0.53	1.66–1	1
84BEN/KUM	298.1	1	0.30	1.724	1.62–1	0.52	1.62–1	1

TABLE 41.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	1.925	1.66–1	0.53	9.75–2	1
Temp. range K		A_1					Level of uncertainty
298.1–298.1		3.12345+1					III

TABLE 41.20.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J $K^{-1}g^{-1}$)	2.198
C_p (J $K^{-1}mol^{-1}$)	259.7

Name: 1–Methoxy–2–propoxyethane
Formula: $C_6H_{14}O_2$

CAS–RN: 17081–22–0
Group No.: 41–021
Molar Mass: 118.18

TABLE 41.21.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73KUS/SUU	298.15	2.106	0.10	not specified		C_p	DDCT	71KON/SUU

Name: 1,1'–Oxybis(2–methoxyethane)
Formula: $C_6H_{14}O_3$

CAS–RN: 111–96–6
Group No.: 41–022
Molar Mass: 134.18

TABLE 41.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
66BEA/CLE	210.0–350.0	16	nosp	99.62	melpt	C_p	BSAO	33SOU/BRI
82VIL/CAS	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
83KIM/DAR	298.1	1	0.30	99.	chrom	C_p	FSIT	71PIC/LED
91NAK/SOE	298.1	1	nosp	99.9	chrom	C_p	FSIO	85OGA
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 41.22.2. Correlated heat capacities

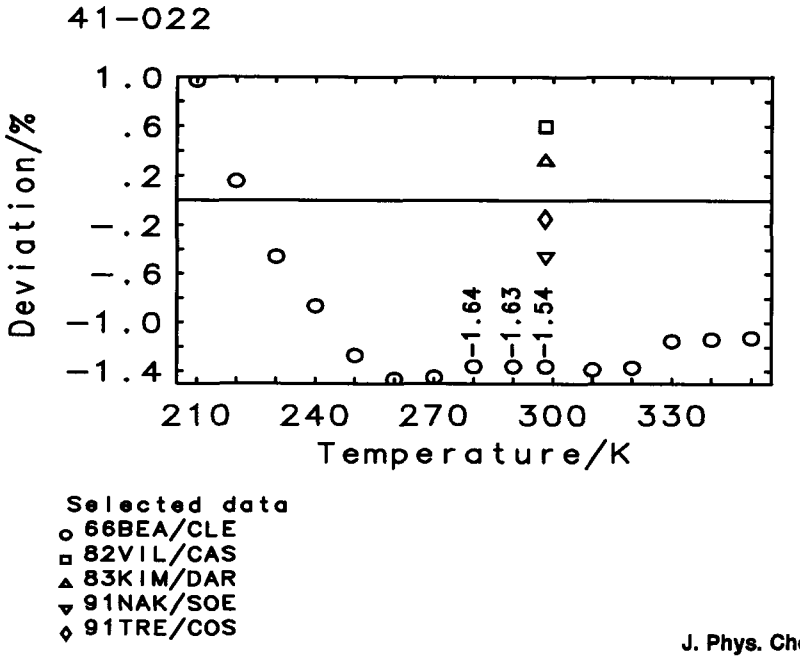
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
66BEA/CLE	210.0–350.0	16	1.50#	0.838	4.14–1	1.26	–3.46–1	–12
82VIL/CAS	298.1	1	0.30	1.982	2.00–1	0.59	2.00–1	1
83KIM/DAR	298.1	1	0.30	1.044	1.05–1	0.31	1.05–1	1
91NAK/SOE	298.1	1	0.50#	0.922	1.54–1	0.46	–1.54–1	–1
91TRE/COS	298.1	1	0.50#	0.300	5.00–2	0.15	–5.00–2	–1

TABLE 41.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.977	3.96–1	1.20	–2.72–1	–12
Temp. range K		A_1	A_2				Level of uncertainty
210.0–350.0		2.95281+1	1.31766				V

TABLE 41.22.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	2.00	2.01	2.02	2.03	2.03	2.04	2.05
C_p (J K^{-1}mol^{-1})	269	270	271	272	273	274	275
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.05	2.06	2.07	2.07	2.07	2.08	2.09
C_p (J K^{-1}mol^{-1})	275	276	277	278	278	279	281
Temp. (K)	330	340	350				
c_p (J K^{-1}g^{-1})	2.10	2.11	2.12				
C_p (J K^{-1}mol^{-1})	282	283	284				



Name: Methoxybenzene
Formula: C_7H_8O

CAS–RN: 100–66–3
Group No.: 41–023
Molar Mass: 108.14

TABLE 41.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH		328.9–350.2	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
02LOU2	N	359.0	1	nosp	not specified		C_{avg}	DSIO	*98LOU
33KOL/UDO		297.1	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
39PHI		304.8	1	nosp	not specified		C_p	BSIO	49WEI
59LUT/PAN		348.0–398.0	eqn	nosp	not specified		C_p	BDHO	58LUT/PAN

02LOU2 average value in temperature range 293–425 K

TABLE 41.23.2. Correlated heat capacities

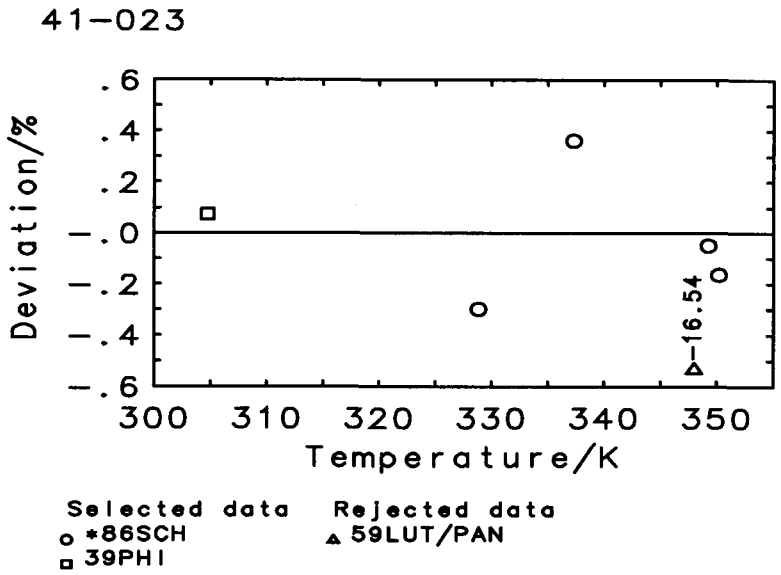
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	328.9–350.2	6	3.00#	0.094	7.02–2	0.28	–2.63–3	–2
39PHI	304.8	1	3.00#	0.024	1.81–2	0.07	1.81–2	1
				Rejected data				
59LUT/PAN	(3.63, 16.54, –3.63, –1)							

TABLE 41.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	7	0.115	8.64–2	0.35	3.32–4	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
304.8–350.2		1.69400+2	–8.98893+1	1.39553+1			VI

TABLE 41.23.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.95	1.91	1.90	1.90	1.93	1.98
C_p ($J\,K^{-1}mol^{-1}$)	211	207	205	206	209	214



Name: 2–Ethoxy–2–methylbutane
Formula: $C_7H_{16}O$

CAS–RN: 919–94–8
Group No.: 41–024
Molar Mass: 116.20

TABLE 41.24.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
36EVA/EDL	298.15	2.092	nosp	not specified	C_p	not specified	

Name: 1–Butoxy–2–methoxyethane
Formula: $C_7H_{16}O_2$

CAS–RN: 13343–98–1
Group No.: 41–025
Molar Mass: 132.20

TABLE 41.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
73KUS/SUU	298.1	1	0.10	not specified	C_p	DDCT	71KON/SUU
91SOE/NAK	298.1	1	nosp	99.9 chrom	C_p	FSIO	85OGA

TABLE 41.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KUS/SUU	298.1	1	0.10	0.403	1.37–2	0.04	1.37–2	1
91SOE/NAK	298.1	1	0.50#	1.997	3.35–1	01.00	–3.35–1	–1

TABLE 41.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	2.037	3.35-1	01.00	-1.61-1	0
Temp. range K		A_1					Level of uncertainty
298.1-298.1		3.39029+1					III

TABLE 41.25.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1} g^{-1}$)	2.132
C_p ($J K^{-1} mol^{-1}$)	281.9

Name: 1,3-Diethoxypropane
Formula: $C_7H_{16}O_2$

CAS-RN: 3459-83-4
Group No.: 41-026
Molar Mass: 132.20

TABLE 41.26.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91SOE/NAK	298.15	2.157	nosp	99.9	chrom	C_p	FSIO	85OGA

Name: 1,5-Dimethoxypentane
Formula: $C_7H_{16}O_2$

CAS-RN: 111-89-7
Group No.: 41-027
Molar Mass: 132.20

TABLE 41.27.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91SOE/NAK	298.15	2.110	nosp	99.9	chrom	C_p	FSIO	85OGA

Name: 1-Ethoxy-4-methoxybutane
Formula: $C_7H_{16}O_2$

CAS-RN: 36865-47-1
Group No.: 41-028
Molar Mass: 132.20

TABLE 41.28.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91SOE/NAK	298.15	2.121	nosp	99.9	chrom	C_p	FSIO	85OGA

Name: 1–Ethoxy–2–propoxyethane
Formula: $C_7H_{16}O_2$

CAS–RN: 18854–31–4
Group No.: 41–029
Molar Mass: 132.20

TABLE 41.29.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91SOE/NAK	298.15	2.104	nosp	99.9	chrom	C_p	FSIO	85OGA

Name: 1–Methoxy–3–propoxypropane
Formula: $C_7H_{16}O_2$

CAS–RN: 89851–49–0
Group No.: 41–030
Molar Mass: 132.20

TABLE 41.30.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91SOE/NAK	298.15	2.110	nosp	99.9	chrom	C_p	FSIO	85OGA

Name: 1,1',1''–[Methylidynetris(oxy)]trisethane
Formula: $C_7H_{16}O_3$

CAS–RN: 122–51–0
Group No.: 41–031
Molar Mass: 148.20

TABLE 41.31.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89JIM/ROU	298.15	1.962	nosp	not specified		C_p	FSIT	71PIC/LED

Name: Ethoxybenzene
Formula: $C_8H_{10}O$

CAS–RN: 103–73–1
Group No.: 41–032
Molar Mass: 122.17

TABLE 41.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	320.0–349.4	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 41.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.001	1.31–3	0.00	9.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
320.0–349.4		1.24794+1	5.11500				V

TABLE 41.32.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J K^{-1} g^{-1}$)	1.96	2.00	2.03	2.07
C ($J K^{-1} mol^{-1}$)	240	244	248	253

Name: 1–Methoxy–4–methylbenzene
Formula: $C_8H_{10}O$

CAS–RN: 104–93–8
Group No.: 41–033
Molar Mass: 122.17

TABLE 41.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	312.2–350.2	7S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 41.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	7	7	0.002	1.59–3	0.01	–5.45–7	0

Temp. range K	A_1	A_2	Level of uncertainty
312.2–350.2	1.31270+1	4.49712	V

TABLE 41.33.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c ($J K^{-1} g^{-1}$)	1.84	1.87	1.90	1.93	1.96
C ($J K^{-1} mol^{-1}$)	225	229	233	236	240

Name: 1,1'–Oxybisbutane
Formula: $C_8H_{18}O$

CAS–RN: 142–96–1
Group No.: 41–034
Molar Mass: 130.23

TABLE 41.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		C_p	not specified	
87COB/CAS		298.1–298.1	2	nosp	99.	anal	C_p	FSIT	71PIC/LED

38PAN/DUD temperature range of parameters validity estimated by the compilers

TABLE 41.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
38PAN/DUD	298.0–362.8	7	5.00#	1.103	2.35	5.52	–5.53–1	–1
87COB/CAS	298.1	2	0.50#	0.199	3.33–2	0.10	3.30–2	2

TABLE 41.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	1.108	2.35	5.52	–4.23–1	1
Temp. range K		A_1	A_2				Level of uncertainty
298.0–362.8		–1.62362+2	6.56661+1				VI

TABLE 41.34.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.21	2.63	3.05	3.47	3.89	4.31	4.73
C_p (J K^{-1}mol^{-1})	288	343	397	452	506	561	616

Name: 1,2–Dipropoxyethane
Formula: $C_8H_{18}O_2$

CAS–RN: 18854–56–3
Group No.: 41–035
Molar Mass: 146.23

TABLE 41.35.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73KUS/SUU	298.15	2.113	0.10	not specified		C_p	DDCT	71KON/SUU

Name: 1,1'–Oxybis(2–ethoxyethane)
Formula: $C_8H_{18}O_3$

CAS–RN: 112–36–7
Group No.: 41–036
Molar Mass: 162.23

TABLE 41.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78ROU/PER1	283.1–313.1	3	0.30	99.8	melpt	C_p	FSIT	71PIC/LED

TABLE 41.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.665	8.35–2	0.20	1.14–4	1
Temp. range K		A_1	A_2				Level of uncertainty
283.1–313.1		3.31510+1	2.92185				III

TABLE 41.36.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.118	2.133	2.146	2.148	2.163
C_p (J K^{-1}mol^{-1})	343.7	346.1	348.1	348.5	350.9

Name: 2,5,8,11–Tetraoxadodecane
Formula: $C_8H_{18}O_4$

CAS–RN: 112–49–2
Group No.: 41–037
Molar Mass: 178.23

TABLE 41.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
66BEA/CLE	230.0–350.0	14	nosp	99.44	melpt	C_p	BSAO	33SOU/BRI
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 41.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
66BEA/CLE	230.0–350.0	14	1.50#	0.049	3.28–2	0.07	1.14–2	5
91TRE/COS	298.1	1	0.50#	0.079	1.76–2	0.04	–1.76–2	–1

TABLE 41.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.061	3.74–2	0.08	9.42–3	4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
230.0–350.0	8.74200+1	–4.20245+1	1.30378+1	–1.27418	V

TABLE 41.37.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.06	2.05	2.05	2.05	2.05	2.05	2.05
C_p (J K^{-1}mol^{-1})	368	366	365	365	365	365	366
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.06	2.06	2.07	2.07	2.09	2.10	2.11
C_p (J K^{-1}mol^{-1})	367	368	368	370	372	374	376
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	2.12						
C_p (J K^{-1}mol^{-1})	378						

TABLE 41.37.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	13	0.142	7.93–2	0.18	9.53–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
250.0–350.0	651.00	5.54117+1	2.27196+1	2.08380+1	3.37865+1	V

Name: 1–Ethoxy–4–mythylbenzene
Formula: $C_9H_{12}O$

CAS–RN: 622–60–6
Group No.: 41–038
Molar Mass: 136.19

TABLE 41.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	320.4–349.9	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 41.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.110	3.65–2	0.11	4.51–5	–2

Temp. range K	A_1	A_2	Level of uncertainty
320.4–349.9	1.42956+1	5.60829	V

TABLE 41.38.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	1.97	2.00	2.04	2.07
C ($J\,K^{-1}mol^{-1}$)	268	273	277	282

Name: 1–Methoxy–2,4–dimethylbenzene
Formula: $C_9H_{12}O$

CAS–RN: 6738–23–4
Group No.: 41–039
Molar Mass: 136.19

TABLE 41.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	322.3–351.0	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 41.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.113	1.09–1	0.34	5.21–4	2

Temp. range K	A_1	A_2	Level of uncertainty
322.3–351.0	1.25781+1	5.86242	V

TABLE 41.39.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	1.91	1.95	1.98	2.02
C ($J\,K^{-1}mol^{-1}$)	261	265	270	275

Name: Propoxybenzene
Formula: $C_9H_{12}O$

CAS–RN: 622–85–5
Group No.: 41–040
Molar Mass: 136.19

TABLE 41.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	320.0–349.3	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 41.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.049	4.82–2	0.15	7.95–5	–2

Temp. range K	A_1	A_2	Level of uncertainty
320.0–349.3	1.25222+1	6.12127	V

TABLE 41.40.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	1.96	2.00	2.04	2.07
C ($J\,K^{-1}mol^{-1}$)	267	272	277	282

Name: 1–Methoxy–4–(1–propenyl)benzene
Formula: $C_{10}H_{12}O$

CAS–RN: 104–46–1
Group No.: 41–041
Molar Mass: 148.20

TABLE 41.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
05LOU	N	401.4	1	nosp	not specified		C_{avg}	DSIO	*98LOU
13NAS/BRE	N	295.6–298.4	3	nosp	not specified		C_p	not specified	

05LOU average value in temperature range 297–506 K
13NAS/BRE error 0.5 % (information in 29WAS)

TABLE 41.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
13NAS/BRE	295.6–298.4	3	3.00#	0.874	1.14	2.62	6.06–2	1

TABLE 41.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	3	1.515	1.98	4.54	6.06–2	1
Temp. range K		A_1	A_2				Level of uncertainty
295.6–298.4		–3.41867+2	1.29435+2				VI

TABLE 41.41.4. Recommended values of heat capacities

Temp. (K)	295	298.15	300
c_p ($J K^{-1}g^{-1}$)	2.24	2.47	2.61
C_p ($J K^{-1}mol^{-1}$)	332	366	386

Name: 1,1'–[1,2–Ethanediylbis(oxy)]bisbutane
Formula: $C_{10}H_{22}O_2$

CAS–RN: 112–48–1
Group No.: 41–042
Molar Mass: 174.28

TABLE 41.42.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.15	2.008	nosp	not specified		C_p	not specified	

52CUR/JOH technical product, purity in question

Name: 1,1'–[Ethylidenebis(oxy)]bisbutane
Formula: $C_{10}H_{22}O_2$

CAS–RN: 871–22–7
Group No.: 41–043
Molar Mass: 174.28

TABLE 41.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
47CON/ELV	298.1–353.1	4S	1.00	99.	anal	C_p	BSIO	49WEI

TABLE 41.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.533	2.29–1	0.53	6.00–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.1–353.1		1.04078+2	–4.24315+1	7.28126			V

TABLE 41.43.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	2.02	2.03	2.04	2.07	2.10	2.14
C_p ($J K^{-1}mol^{-1}$)	352	353	356	360	366	372

Name: 2,5,8,11,14–Pentaoxapentadecane
Formula: $C_{10}H_{22}O_5$

CAS–RN: 143–24–8
Group No.: 41–044
Molar Mass: 222.28

TABLE 41.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65KRI/LOE	293.0–426.1	13	nosp	99.5	chrom	C_p	not specified	
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 41.44.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65KRI/LOE	293.0–426.1	13	2.00#	0.364	4.21–1	0.73	–7.13–3	–1
91TRE/COS	298.1	1	0.50#	0.038	1.06–2	0.02	1.06–2	1

TABLE 41.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.379	4.38–1	0.76	–5.87–3	0
Temp. range K		A_1	A_2				Level of uncertainty
293.0–426.1		4.04616+1	4.86469				V

TABLE 41.44.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.04	2.06	2.06	2.08	2.10	2.11	2.13
C_p (J K^{-1}mol^{-1})	454	457	458	462	466	470	474
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.15	2.17	2.19	2.20	2.22	2.24	2.26
C_p (J K^{-1}mol^{-1})	478	482	486	490	494	498	502
Temp. (K)	420	430					
c_p (J K^{-1}g^{-1})	2.28	2.30					
C_p (J K^{-1}mol^{-1})	506	510					

TABLE 41.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.407	3.87–1	0.68	3.97–2	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
293.0–426.1	705.00	7.76270+1	1.00481+1	1.66259+1	1.49928+2	V

Name: 1–Methoxydecane
Formula: $C_{11}H_{24}O$

CAS–RN: 7289–52–3
Group No.: 41–045
Molar Mass: 172.31

TABLE 41.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75AND/MAR	246.5–349.3	38	nosp	99.65	melpt	C_p	BSAO	63AND/COU1

TABLE 41.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	38	0.334	2.98–2	0.07	3.79–5	–4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
246.5–349.3	1.28794+2	–8.91507+1	2.94601+1	–3.02968	II

TABLE 41.45.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.061	2.070	2.085	2.091	2.105	2.129	2.151
C_p (J K^{-1}mol^{-1})	355.1	356.7	359.3	360.3	362.8	366.9	370.6

Temp. (K)	300	310	320	330	340	350	
c_p (J K^{-1}g^{-1})	2.156	2.185	2.215	2.246	2.276	2.304	
C_p (J K^{-1}mol^{-1})	371.5	376.5	381.7	387.0	392.1	397.1	

TABLE 41.45.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	38	1.047	9.28–2	0.21	3.45–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
246.5–349.3	652.20	5.06054+1	3.12092+1	8.60490	2.05141+1	II

Name: 1,1'–Oxybisbenzene
Formula: $C_{12}H_{10}O$

CAS–RN: 101–84–8
Group No.: 41–046
Molar Mass: 170.21

TABLE 41.46.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
51FUR/GIN	N	300.0–570.0	28S	nosp	99.993	melpt	C_{sat}	DSTO	50GIN/DOU
79YUE/YOS		323.1–463.1	8	2.00	not specified		C_{sat}	BDHT	71DU/COM
86MER/BEN		305.9–370.5	14	nosp	not specified		C_p	BDCT	86MER/BEN
87MIL/FEN1		323.1–423.1	6	1.50	not specified		C_p	BDHT	87PER/COM

51FUR/GIN same data in 53GIN/FUR; adiabatic calorimeter 45SCO/MEY used above 360 K

TABLE 41.46.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
51FUR/GIN	300.0–570.0	28	0.10#	0.206	7.66–3	0.02	2.32–6	0
				Rejected data				
79YUE/YOS	(6.99–1, 1.80, 6.76–1, 8)			86MER/BEN	(3.85–1, 1.13, 3.36–1, 14)			
87MIL/FEN1	(4.14–1, 1.16,–3.86–1, –6)							

TABLE 41.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	56	28	0.218	8.10–3	0.02	2.32–6	0
C_{sat}	56	28	0.205	6.96–3	0.02	2.32–6	–2

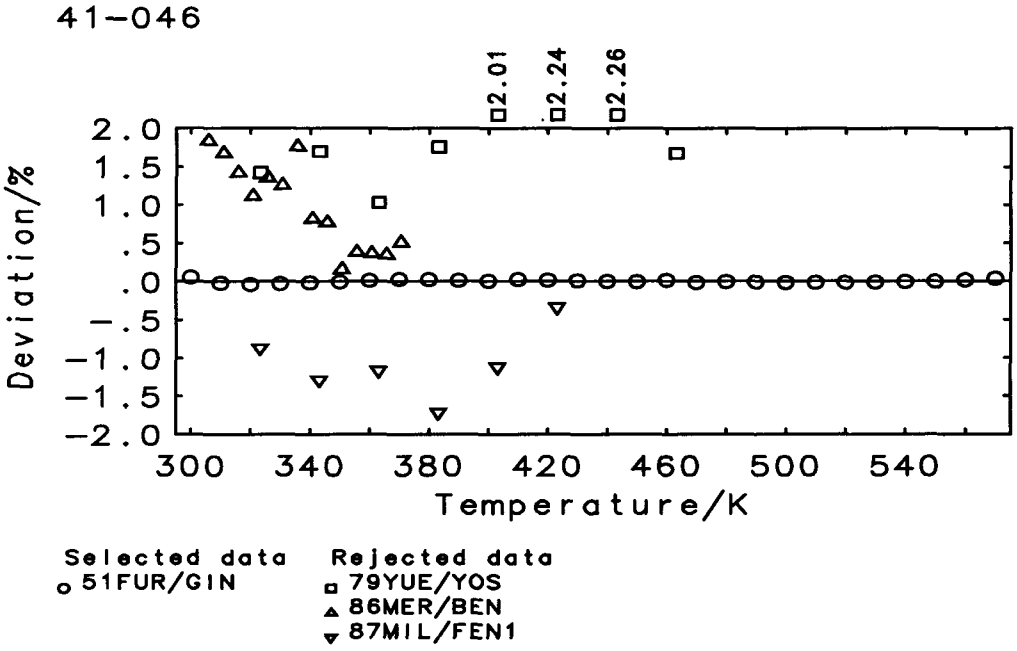
Temp. range K	A_1	A_2	A_3	Level of uncertainty
300.0–570.0	1.58924+1	5.48559	–9.44220–3	II
300.0–570.0	1.56219+1	5.63025	–2.83961–2	II

TABLE 41.46.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p ($J\,K^{-1}g^{-1}$)	1.576	1.603	1.629	1.656	1.682	1.709	1.735
C_p ($J\,K^{-1}mol^{-1}$)	268.3	272.8	277.3	281.8	286.3	290.8	295.3
c_{sat} ($J\,K^{-1}g^{-1}$)	1.576	1.602	1.629	1.656	1.682	1.709	1.735
C_{sat} ($J\,K^{-1}mol^{-1}$)	268.2	272.7	277.3	281.8	286.3	290.8	295.4
Temp. (K)	370	380	390	400	410	420	430
c_p ($J\,K^{-1}g^{-1}$)	1.761	1.788	1.814	1.841	1.867	1.894	1.920
C_p ($J\,K^{-1}mol^{-1}$)	299.8	304.3	308.8	313.3	317.8	322.3	326.8
c_{sat} ($J\,K^{-1}g^{-1}$)	1.762	1.788	1.815	1.841	1.867	1.894	1.920
C_{sat} ($J\,K^{-1}mol^{-1}$)	299.9	304.4	308.9	313.4	317.9	322.3	326.8
Temp. (K)	440	450	460	470	480	490	500
c_p ($J\,K^{-1}g^{-1}$)	1.946	1.973	1.999	2.026	2.052	2.078	2.105
C_p ($J\,K^{-1}mol^{-1}$)	331.3	335.8	340.3	344.8	349.3	353.7	358.2
c_{sat} ($J\,K^{-1}g^{-1}$)	1.946	1.973	1.999	2.025	2.051	2.077	2.104
C_{sat} ($J\,K^{-1}mol^{-1}$)	331.3	335.8	340.2	344.7	349.1	353.6	358.0
Temp. (K)	510	520	530	540	550	560	570
c_p ($J\,K^{-1}g^{-1}$)	2.131	2.157	2.184	2.210	2.236	2.262	2.289
C_p ($J\,K^{-1}mol^{-1}$)	362.7	367.2	371.7	376.1	380.6	385.1	389.6
c_{sat} ($J\,K^{-1}g^{-1}$)	2.130	2.156	2.182	2.208	2.234	2.260	2.286
C_{sat} ($J\,K^{-1}mol^{-1}$)	362.5	366.9	371.4	375.8	380.2	384.6	389.0

TABLE 41.46.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	56	28	0.227	8.53–3	0.02	–1.63–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
300.0–570.0	766.80	1.77945–1	1.89106–4	1.59769+1	4.18605+1		II



Name: 1,1'–[Oxybis(2,1–ethanediyloxy)]bisbutane
Formula: $C_{12}H_{26}O_3$

CAS–RN: 112–73–2
Group No.: 41–047
Molar Mass: 218.34

TABLE 41.47.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.15	1.799	nosp	not specified	C_p	not specified	

52CUR/JOH technical product, purity in question

Name: 1,4–Bis(1,1–diethoxyethyl)benzene
Formula: $C_{18}H_{30}O_4$

CAS–RN: 47189–08–2
Group No.: 41–048
Molar Mass: 310.43

TABLE 41.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
78KAR/RAB		326.6–340.0	2	nosp	not specified	C_p	BSAO	76LEB/LIT
78KAR/SAP	N	331.3–341.3	2	0.20	98.94 melpt	C_p	BSAO	76LEB/LIT

78KAR/SAP data from a graph only

TABLE 41.48.2. Correlated heat capacities

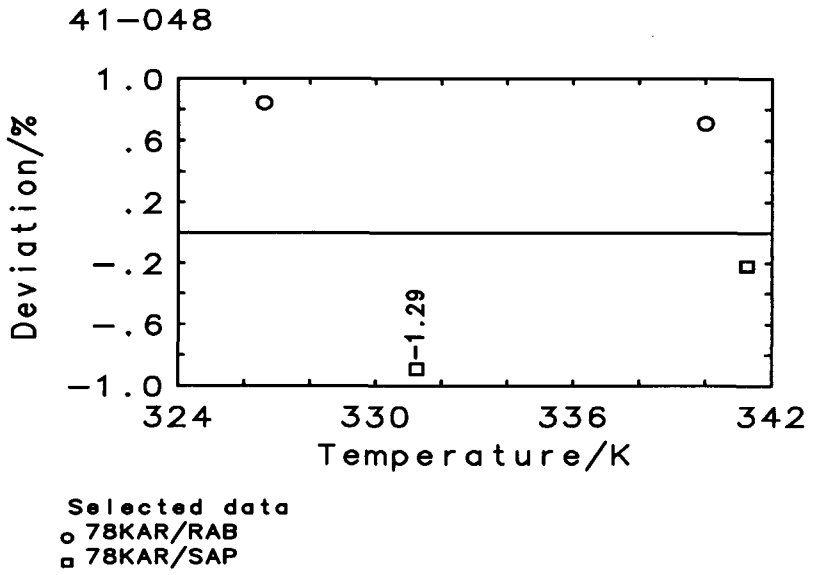
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
78KAR/RAB	326.6–340.0	2	0.70#	1.108	5.58–1	0.78	5.56–1	2
78KAR/SAP	331.3–341.3	2	0.70#	1.328	6.54–1	0.93	–5.35–1	–2

TABLE 41.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.729	8.60–1	1.21	1.04–2	0
Temp. range K		A_1	A_2				Level of uncertainty
326.6–341.3		3.64411+1	1.05145+1				IV

TABLE 41.48.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p (J K^{-1}g^{-1})	1.905	1.934
C_p (J K^{-1}mol^{-1})	591.5	600.2



42. Alcohols and Phenols

The family of alcohols and phenols contains 105 compounds, of which 26 compounds were measured at one temperature only (mainly 298.15 K). The frequency of measurements was the highest for 1-alkanols which corresponds to the importance of these compounds for technology and industry. The data for 1-alkanols C_1 do C_{18} have been recently evaluated and the recommended values have been published in the review article by Zábranský et al. (90ZAB/RUZ). These values are also the basis of recommendations in this monograph.

A large number of important alcohols and phenols were studied at NPLT and consist of the following: isomeric propanols (63AND/COU2, 68COU/LEE), isomeric butanols (65COU/HAL, 68COU/LEE, 71AND/CON), 1-pentanol (68COU/LEE), phenol (63AND/COU1) and three isomers of methylphenols (cresols) (67AND/COU). Results of these accurate measurements served in all cases as the basis for our recommendations. The above data have been complemented by the high temperature data from GPI (67RAS/GAN, 79GRI/YAN) which are available for eight 1-alkanols, phenol, and benzenemethanol.

Beside the NPLT measurements, a significant number of determinations for this family were performed in 1920's and 1930's at SUC, YUNH and JHUB. These data have been included in the final selection in those cases where values of higher quality were not available and consist of: 14 octanol isomers and benzenemethanol measured at JHUB (31CLI/AND, 31SMI/AND1), three benzenediols and two naphthols studied at YUNH (26AND/LYN) and measurements from SUC for ethylene glycol (25PAR/KEL), 1,2-propanediol (27PAR/HUF), erythritol and D-mannitol (32SPA/THO), 2-methyl-2-butanol (33PAR/HUF), benzenemethanol (36PAR/TOD1), and 1-heptanol and cyclopentanol (56PAR/KEN).

Equations expressing heat capacity for 4 isomeric pentanols as a first degree polynomial in the temperature over an interval of 30 K (estimated reliability is about 2 %) were published by Lee at ULE (49LEE). Five branched unsaturated alcohols important for the pharmaceutical industry were measured over a narrow temperature interval at BTIM (84BAG/BAE, 86BER/GUR).

Additional high quality results were obtained for cyclohexanol and cycloheptanol at UOTO (68ADA/SUG, 72ADA/SUG).

The largest number of reliable data sets is available for C_1 to C_3 alkanols. In the case of methanol, the recommended data have been established by combining the following three sources: the low temperature measurements from UMAA (71CAR/WES), the data near the normal boiling temperature from NBSW (31FIO/GIN), and the high-pressure values up to the critical temperature from UMF (88BOY/CRI). The latter data set has been converted to saturated liquid conditions using the procedure described in detail in the literature (90ZAB/RUZ). The equation of state for liquid methanol (83MAC/STR) has been used in combination with vapor pressure data calculated from the Wagner equation with the parameters reported by McGarry (83MCG).

Recommended data for ethanol are based mainly on the three low-temperature data sets measured at UOTO (77HAI/SUG2) and GITA (66HWA/ZIE, 79BRO/ZIE) as well as two sets of values close to the normal boiling temperature from NBSW (31FIO/GIN) and UGG (66KLE).

For all isomeric propanols and butanols (with the exception of 2-methyl-2-butanol which was not studied at NPLT), the principle data source has been measurements from NPLT and consist of the following: 1-propanol (68COU/LEE), 2-propanol (63AND/COU2), 1-butanol (65COU/HAL), 2-butanol (71AND/CON), 2-methyl-1-butanol (68COU/LEE). For 1-propanol this source has been complemented by low-temperature data determined at PASW (80KAL/JED) and high-temperature data from UGG (51EUC/EIG) and GPI (79GRI/YAN). For 2-propanol the additional sources were measurements from GITA (79BRO/ZIE, available only in the form of $C_p = C_p(T)$ equation) and high-temperature values from NBSW (48GIN/COR) reliable to 0.8 %. In the final correlation, the high temperature data for 1-butanol from MITC (75SAN) and GPI (79GRI/YAN) have also been used. The only reliable sources for 2-methyl-2-butanol are those of Oetting at DCM (63OET) and the work from MITC (77HOF/SAN) which covers higher temperatures. Reliable data for 2-butanol are available for compounds with specified chiralities for which we have developed recommended values. Data for 2-butanol with an unspecified chirality have not been evaluated as only two sets of low reliability data were published. There is only the table of Experimental Heat Capacity for this compound.

In the case of the pentanols, multiple measurements are available only for 1-pentanol. Recommended values have been based on accurate data from NPLT (68LEE/COU) and also on high-temperature data from GPI (79GRI/YAN). Although there are a relatively large number of data sets available for C_6 to C_8 alkanols, the agreement among these sets is low. It was very difficult to decide which data should be included in the final correlation. For that reason, some verification experiments were performed at ICTP (89VES/BAR) which have been included and helped in the final selection of the data sets. The following sources have been selected: 1-hexanol, data sets from PASW (84KAL/WOY) and UCB (29KEL2); 1-heptanol, measurements from SUC (56PAR/KEN); 1-octanol, two data sets from JHUB (31CLI/AND, 61ROU, 89VES/BAR). In the case of 1-hexanol, the high-temperature data from GPI have also been used (79GRI/YAN).

Mainly the data from the laboratories in fSU were available for higher 1-alkanols. Particularly active were the authors from SRIL (80VAS/TRE, 82VAS/PET) who published results in the form of parameters of a correlating equation $C_p = C_p(T)$. Our experience tells us that their reliability is not very good (experimental error around 2 %). For measurements performed for higher 1-alkanols, one finds the results from ULS (79SVE) for 1-decanol and 1-dodecanol and those from FUAN (74MOS/MOU) for C_{13} to C_{16} 1-alkanols. The recommended data have, however, high level of uncertainty considering the uncertain quality of data in the primary sources. We have not found any primary data for higher aliphatic 1-alkanols than C_{18}.

Among the alkanediols, the most frequently measured substance has been ethylene glycol for which 10 references are available and provide data as a function of temperature. From these references, four data sets were selected as the basis for the recommended values, two from CIUG (62RAB/NIK, 67NIK/RAB1), one older measurement from SUC (25PAR/KEL), and one from UCCW (79STE/TEM) in which extensive data were given for temperatures up to 493 K having a reported uncertainty 1 %. The only two data sources for 1,2-propanediol were older measurements from SUC (25PAR/KEL) and secondary data from a monograph called "Glycols" edited by Curme (52CUR). The secondary data were obtained by combining the Dow Chemical and Union Carbide measurements (not available in open literature) with the above data from SUC. One data set is available for 1,4- and 2,3-butanediols; the data from CIUG (79NIS/BAB) for the 1,4- isomer can be considered as reliable while the data from a unidentified laboratory in fSU (36KHO/KAL) are highly doubtful. The latter measurements were obtained using drop calorimetry and yielded average heat capacities. The correction for curvature was applied showing the quadratic temperature dependence of the true heat capacity. This explains why the deviations of the correlation are equal zero for this compound.

The best known alkanetriol is certainly glycerol for which 11 data sources are available, however, most sources report data only near room temperatures. The measurements from CIUG (62RAB/NIK) as well as the secondary data of Omel'chenko (62OME) served as the basis for the recommended values. The secondary data of Omel'chenko which extend to temperatures up to 353 K are based on various primary fSU values determined in the 1950's (unavailable for us) and also some older data (*79BER). Assignment of the level of uncertainty V reflects the dubious origin of some of the data used in this correlation.

Data for cycloalkanols show only two sources available for cyclopentanol and cycloheptanol, and two data sets for cyclohexanol. For cyclohexanol, the first set contains reliable measurements over an interval of 16 K measured at UOTO (68ADA/SUG) and the second data set provides extensive data up to 428 K from LCPP (74PET/TER). The only measurement on cycloheptanol comes from UOTO (72ADA/SUG).

Several aromatic alcohols, phenol and three cresols were carefully investigated at NPLT (63AND/COU1, 67AND/COU). In the case of phenol, the values measured up to 373 K from GPI (67RAS/GAN) were included for establishing the final recommended values. The measurements on three benzenediols at YUNH and measurements on benzenemethanol from JHUB have already been mentioned above.

Special attention was paid to deuterated ethanol, ethylene glycol and glycerol at CIUG (62RAB/NIK, 67NIK/RAB1, 67NIK/RAB2), while the deuterated methanol was studied at ICLO (49STA/GUP).

Name: Methanol-*d*
Formula: CH_3DO

CAS-RN: 1455-13-6
Group No.: 42-001
Molar Mass: 33.05

TABLE 42.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49STA/GUP	180.0–270.0	10	0.50	not specified		C_p	BSAO	49STA/GUP

TABLE 42.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.597	2.63-2	0.30	9.66-5	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.0–270.0		-8.99853	2.41876+1	-1.11447+1	1.75346		IV

TABLE 42.1.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1}g^{-1}$)	2.178	2.202	2.220	2.236	2.250	2.267	2.289
C_p ($J K^{-1}mol^{-1}$)	71.98	72.77	73.38	73.88	74.37	74.93	75.65
Temp. (K)	250	260	270				
c_p ($J K^{-1}g^{-1}$)	2.318	2.357	2.409				
C_p ($J K^{-1}mol^{-1}$)	76.61	77.91	79.62				

Name: Methanol
Formula: CH_4O

CAS–RN: 67–56–1
Group No.: 42–002
Molar Mass: 32.04

TABLE 42.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
07WAL		292.1	1	nosp	not specified	C_{avg}	DSIO	07WAL
25DRU/WEI		293.1	1	nosp	not specified	C_p	BSIO	25DRU/WEI
25PAR		188.4–290.1	8	0.50	not specified	C_p	BSIO	25PAR
29KEL1		181.1–292.0	14	1.00	not specified	C_p	BSIO	29KEL1
29MIT/HAR1		190.5–264.8	18	nosp	not specified	C_p	BSIO	29MIT/HAR1
31FIO/GIN	N	318.1–378.1	7S	0.10	99.97 estim	C_{sat}	BSIO	31FIO/GIN
39PHI		300.8	1	nosp	not specified	C_p	BSIO	49WEI
49STA/GUP		180.0–270.0	10S	0.50	not specified	C_p	BSAO	49STA/GUP
49TSC/RIC2		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
50HOU/MAS2		323.1–353.1	4S	0.40	99.8 estim	C_p	BSAO	50SAG/HOU
60SWI/ZIE	N	311.6	1	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
62KAT		283.1–333.1	4	nosp	not specified	C_p	BSIO	62KAT
66DRA/LAN	N	298.1	1	nosp	not specified	C_p	BSIO	66DRA/LAN
68PAZ/REC	N	313.1	1	nosp	not specified	C_p	BDCT	70PAZ/PAZ
71CAR/WES		180.0–320.0	17S	nosp	99.975 melpt	C_p	BSAO	68WES/FUR
71DES/BHA		298.1–318.1	3S	1.00	not specified	C_p	BSIO	56MUR/VAN
71GOP/GAM		308.0–333.0	eqn	1.00	not specified	C_p	BSAO	71GOP/GAM
81ATA/ELS		293.1	1	2.50	not specified	C_p	BDHO	81ATA/ELS
82BEN/DAR		288.1–308.1	2	nosp	not specified	C_p	FSIT	71PIC/LED
82VIL/CAS		298.1	1	0.30	99.8 chrom	C_p	FSIT	71PIC/LED
84ZEG/SOM2		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
85COS/PAT8		298.1–313.1	2	nosp	not specified	C_p	FSIT	71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified	C_p	BSAO	83KUK/KOR
86OGA/MUR		298.1	1	0.10	not specified	C_p	FSIO	85OGA
86TAN/TOY		298.1	1	0.30	99.96 anal	C_p	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FSIT	71PIC/LED
88BOY/CRI	N	393.1–503.1	5	nosp	not specified	C_p	FSIO	87LAN/CRI
88OKA/OGA	N	298.1–299.1	2	nosp	not specified	C_p	FSIO	85OGA
89DOU/KHA		298.1	1	nosp	99.8 estim	C_p	FSIT	71PIC/LED

31FIO/GIN data calculated using procedure by 85WIL/CHA
60SWI/ZIE average value in temperature range 294–329 K
66DRA/LAN grade: pure, water content 0.08 %
68PAZ/REC same datum in 70PAZ/PAZ
88BOY/CRI original data measured at 8.3 MPa converted to vapour pressure
88OKA/OGA water content below 0.083 mol.%

TABLE 42.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31FIO/GIN	318.1–378.1	7	0.20#	1.724	3.59–2	0.34	–1.98–2	–3
71CAR/WES	180.0–320.0	17	0.10#	0.737	7.42–3	0.07	1.98–3	3
88BOY/CRI	393.1–503.1	5	3.00#	1.404	7.40–1	4.21	3.54–1	1
				Rejected data				
07WAL	(1.01–1, 1.04, 1.01–1, 1)			25DRU/WEI	(1.95–1, 2.06,–1.95–1, –1)			
25PAR	(2.64–2, 0.29, 9.33–3, 4)			29KEL1	(6.34–2, 0.74,–5.38–2, –12)			
29MIT/HAR1	(2.88–1, 3.13, 2.46–1, 16)			39PHI	(6.17–1, 5.91, 6.17–1, 1)			
49STA/GUP	(6.16–2, 0.71,–4.08–2, –4)			49TSC/RIC2	(2.42–1, 2.42, 2.42–1, 1)			
50HOU/MAS2	(1.01–1, 0.89, 7.28–2, 2)			60SWI/ZIE	(3.59–1, 3.69, –3.59–1, –1)			
62KAT	(7.11–1, 6.52, 6.92–1, 4)			66DRA/LAN	(1.56–1, 1.58, 1.56–1, 1)			
68PAZ/REC	(1.95–1, 1.89, 1.95–1, 1)			71DES/BHA	(3.66–1, 3.51, 3.63–1, 3)			
71GOP/GAM	(6.74–1, 6.93,–6.63–1, –3)			81ATA/ELS	(7.95–2, 0.82, 7.95–2, 1)			
82BEN/DAR	(6.38–2, 0.64, 1.41–2, 0)			82VIL/CAS	(9.76–2, 0.99, 9.76–2, 1)			
84ZEG/SOM2	(4.34–2, 0.44, 4.34–2, 1)			85COS/PAT8	(1.15–1, 1.17, –1.15–1, –2)			
86KOR/KUK	(5.87–2, 0.62, 5.33–2, 2)			86OGA/MUR	(9.97–2, 1.03, –9.97–2, –1)			
86TAN/TOY	(5.43–2, 0.55, 5.43–2, 1)			88AND/PAT	(1.05–1, 1.08, –1.05–1, –1)			
88OKA/OGA	(9.13–2, 0.94,–9.13–2, –2)			89DOU/KHA	(1.23–2, 0.13, 1.23–2, 1)			

TABLE 42.2.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	115	29	1.317	3.46–1	1.97	5.74–2	1
C_{sat}	115	29	1.547	6.27–1	3.03	9.69–2	3

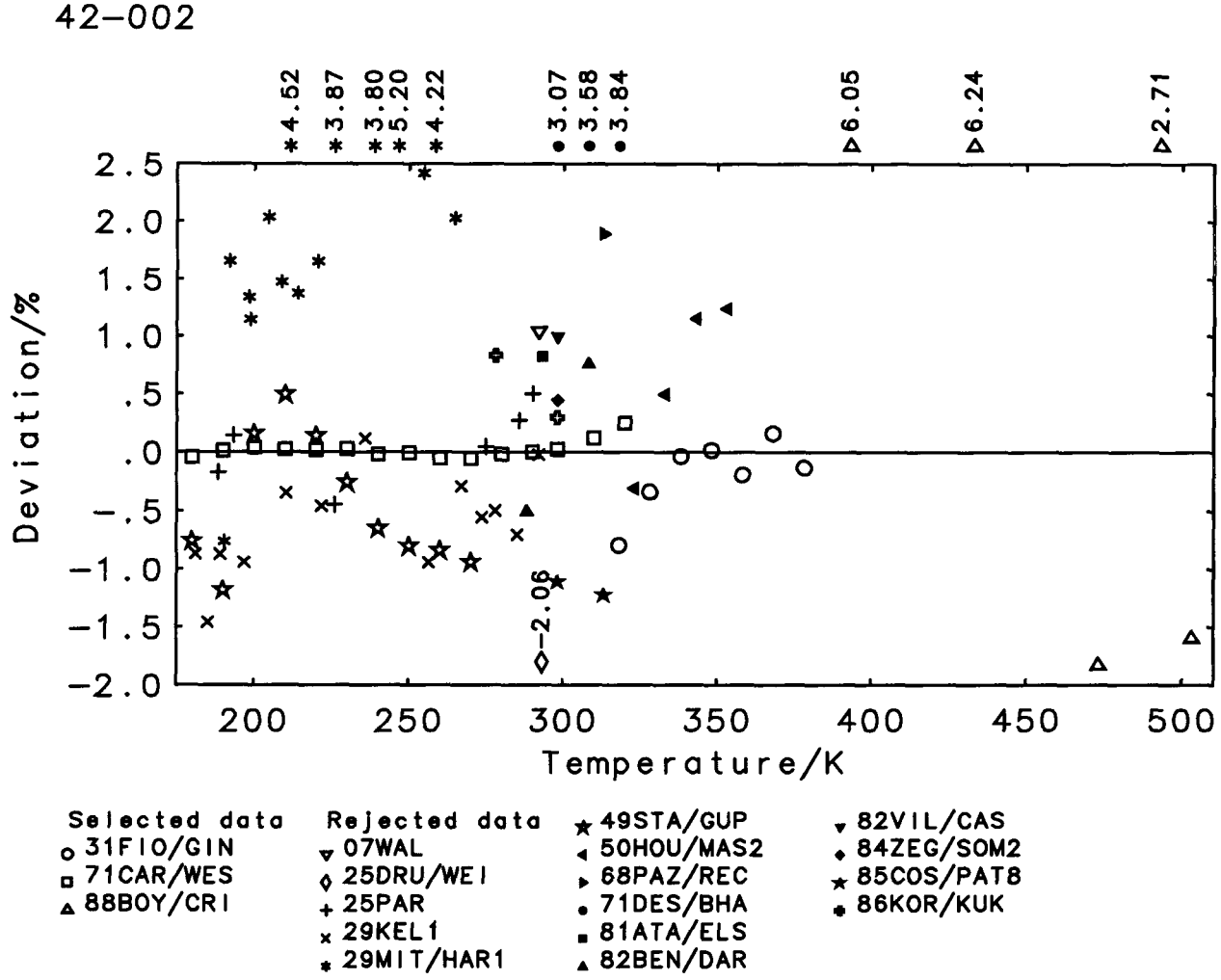
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
180.0–300.0	1.11400+1	–2.60658	5.13940–1	6.85963–2	II
300.0–400.0	7.43918	1.09421	–7.19654–1	2.05662–1	III
400.0–503.1	–5.32654+2	4.06164+2	–1.01987+2	8.64462	V
180.0–300.0	1.14325+1	–2.98427	6.73849–1	4.63833–2	II
300.0–400.0	6.91049	1.53778	–8.33502–1	2.13867–1	III
400.0–503.1	–1.73752+2	1.37035+2	–3.47077+1	3.03672	VI

TABLE 42.2.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J\,K^{-1}g^{-1}$)	2.209	2.209	2.214	2.223	2.238	2.257	2.282
C_p ($J\,K^{-1}mol^{-1}$)	70.78	70.78	70.93	71.24	71.70	72.32	73.11
c_{sat} ($J\,K^{-1}g^{-1}$)	2.209	2.209	2.214	2.223	2.237	2.257	2.282
C_{sat} ($J\,K^{-1}mol^{-1}$)	70.80	70.78	70.93	71.23	71.69	72.32	73.11
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J\,K^{-1}g^{-1}$)	2.311	2.346	2.387	2.401	2.433	2.485	2.531
C_p ($J\,K^{-1}mol^{-1}$)	74.06	75.19	76.49	76.93	77.96	79.62	81.11
c_{sat} ($J\,K^{-1}g^{-1}$)	2.312	2.347	2.387	2.401	2.433	2.485	2.531
C_{sat} ($J\,K^{-1}mol^{-1}$)	74.07	75.20	76.50	76.94	77.97	79.62	81.10
Temp. (K)	300	310	320	330	340	350	360
c_p ($J\,K^{-1}g^{-1}$)	2.542	2.606	2.675	2.752	2.835	2.925	3.022
C_p ($J\,K^{-1}mol^{-1}$)	81.46	83.50	85.73	88.17	90.82	93.71	96.84
c_{sat} ($J\,K^{-1}g^{-1}$)	2.542	2.605	2.674	2.749	2.831	2.920	3.016
C_{sat} ($J\,K^{-1}mol^{-1}$)	81.46	83.47	85.68	88.08	90.71	93.55	96.64
Temp. (K)	370	380	390	400	410	420	430
c_p ($J\,K^{-1}g^{-1}$)	3.128	3.241	3.363	3.494	3.64	3.80	4.00
C_p ($J\,K^{-1}mol^{-1}$)	100.2	103.9	107.8	111.9	116	122	128
c_{sat} ($J\,K^{-1}g^{-1}$)	3.120	3.232	3.352	3.481	3.62	3.77	3.94
C_{sat} ($J\,K^{-1}mol^{-1}$)	99.96	103.5	107.4	111.5	116	121	126
Temp. (K)	440	450	460	470	480	490	500
c_p ($J\,K^{-1}g^{-1}$)	4.25	4.56	4.95	5.43	6.01	6.71	7.54
C_p ($J\,K^{-1}mol^{-1}$)	136	146	159	174	193	215	242
c_{sat} ($J\,K^{-1}g^{-1}$)	4.14	4.36	4.61	4.90	5.24	5.62	6.05
C_{sat} ($J\,K^{-1}mol^{-1}$)	133	140	148	157	168	180	194

TABLE 42.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	115	29	3.428	6.60–1	2.75	1.99–1	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
180.0–503.1	512.64	–3.21671	7.19427–2	8.09368	–8.23642–1	–1.44020+1	2.04604+1	V



Name: 1,2–Ethanediol–d_2
Formula: $C_2H_4D_2O_2$

CAS–RN: 2219–52–5
Group No.: 42–003
Molar Mass: 64.08

TABLE 42.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62RAB/NIK	N	283.1–328.1	10S	0.30	not specified		C_p	BSAO	47SKU
67NIK/RAB1		265.0–310.0	10S	0.30	not specified		C_p	BSAO	56POP/KOL

62RAB/NIK sample deuterated to 97–98 mol.%

TABLE 42.3.2. Correlated heat capacities

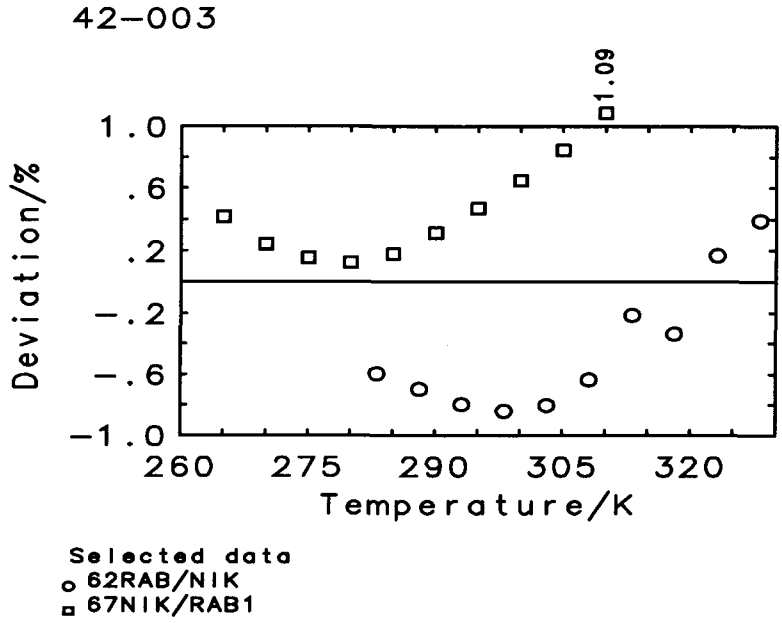
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62RAB/NIK	283.1–328.1	10	0.30	2.001	1.13–1	0.60	–8.17–2	–6
67NIK/RAB1	265.0–310.0	10	0.30	1.803	1.04–1	0.54	8.43–2	10

TABLE 42.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	20	20	2.007	1.15–1	0.60	1.30–3	4
Temp. range K		A_1	A_2				Level of uncertainty
265.0–328.1		5.11629	4.62753				IV

TABLE 42.3.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.225	2.285	2.304	2.345	2.405	2.454	2.465
C_p (J K^{-1}mol^{-1})	142.6	146.4	147.6	150.3	154.1	157.3	158.0
Temp. (K)	310	320	330				
c_p (J K^{-1}g^{-1})	2.525	2.585	2.645				
C_p (J K^{-1}mol^{-1})	161.8	165.7	169.5				



Name: Ethanol–*d*
Formula: C_2H_5DO

CAS–RN: 925–93–9
Group No.: 42–004
Molar Mass: 47.08

TABLE 42.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62RAB/NIK	N	288.1–328.1	9S	0.30	not specified		C_p	BSAO	47SKU
67NIK/RAB2	N	160.0–250.0	19S	0.20	not specified		C_p	BSAO	56POP/KOL

62RAB/NIK sample deuterated to 97–98 mol.%
67NIK/RAB2 sample deuterated to 98 mol.%

TABLE 42.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62RAB/NIK	288.1–328.1	9	0.30	1.930	7.92–2	0.58	–1.94–2	1
67NIK/RAB2	160.0–250.0	19	0.20	0.833	1.97–2	0.17	4.39–3	0

TABLE 42.4.3. Parameters of regression polynomial

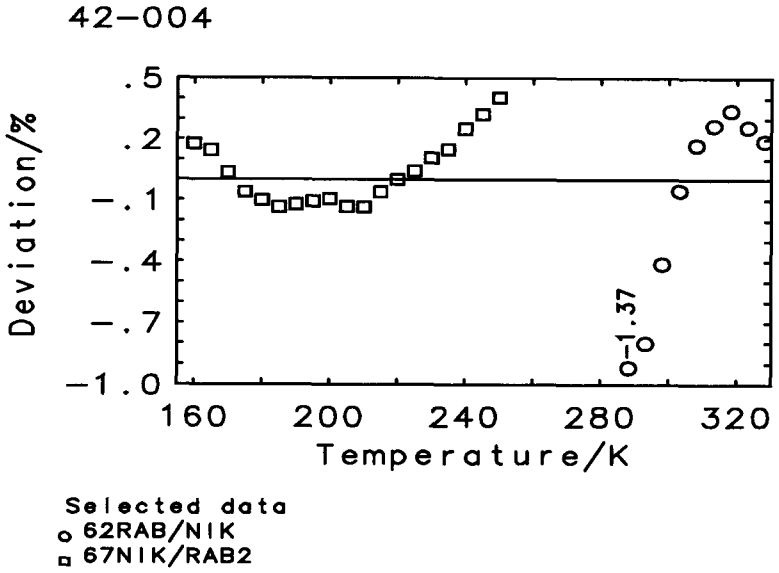
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	28	1.395	5.16–2	0.38	–3.27–3	1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
160.0–328.1	9.59223	2.03173	–1.47816	4.34937–1			III

TABLE 42.4.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J K^{-1} g^{-1}$)	1.915	1.927	1.942	1.960	1.982	2.008	2.038
C_p ($J K^{-1} mol^{-1}$)	90.13	90.72	91.43	92.29	93.31	94.52	95.94
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	2.073	2.114	2.160	2.213	2.272	2.292	2.338
C_p ($J K^{-1} mol^{-1}$)	97.59	99.50	101.7	104.2	106.9	107.9	110.1
Temp. (K)	290	298.15	300	310	320	330	
c_p ($J K^{-1} g^{-1}$)	2.413	2.479	2.495	2.586	2.686	2.796	
C_p ($J K^{-1} mol^{-1}$)	113.6	116.7	117.5	121.7	126.5	131.6	

TABLE 42.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	28	1.571	4.69–2	0.37	3.27–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
160.0–328.1	515.10	1.54399+1	9.95245	2.29518–1	5.98821		III



Name: Ethanol
Formula: C_2H_6O

CAS–RN: 64–17–5
Group No.: 42–005
Molar Mass: 46.07

TABLE 42.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
07WAL		291.6	1	nosp	not specified		C_{avg}	DSIO	07WAL
20GIB/PAR		196.2–271.4	11	nosp	not specified		C_p	BSIO	20GIB/LAT
24WIL/DAN		300.0–332.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
25PAR	N	160.0–298.0	7S	0.50	not specified		C_p	BSIO	25PAR
29KEL2		163.5–294.3	20	1.00	99.96	estim	C_p	BSIO	29KEL1
29MIT/HAR1		184.4–268.8	25	nosp	not specified		C_p	BSIO	29MIT/HAR1
31BLA/LEI		303.1–343.1	9	3.00	not specified		C_p	BSIO	31BLA/LEI
31FIO/GIN	N	318.1–378.1	7S	0.10	not specified		C_{sat}	BSIO	31FIO/GIN
36ERN/WAT		298.1	1	nosp	not specified		C_p	BSIO	49WEI
39BYK		298.1	1	nosp	not specified		C_p	BSIT	39BYK
49TSC/RIC2		298.1	1	nosp	not specified		C_p	BSIO	49TSC/RIC1
60SWI/ZIE	N	316.5	1	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1
62RAB/NIK		288.1–328.1	9S	0.30	not specified		C_p	BSAO	47SKU
65KAU/BIT		293.1–349.1	11	1.00	not specified		C_p	FSIO	65KAU/BIT
66HWA/ZIE		165.3–304.2	41	nosp	99.95	chrom	C_p	BSAO	45SCO/MEY
66KLE		293.1–343.1	11S	0.10	not specified		C_p	BSAO	66KLE
67GRA		308.1–338.1	6	1.00	not specified		C_p	BSIO	67GRA
67NIK/RAB2		160.0–250.0	19S	0.20	not specified		C_p	BSAO	56POP/KOL
68PAZ/REC	N	313.1	1	nosp	not specified		C_p	BDCT	70PAZ/PAZ
75PED/KAY		300.8–344.2	16	nosp	not specified		C_p	BSIO	75PED/KAY

TABLE 42.5.1. Experimental heat capacities Continued

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
76FOR/BEN1		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
77HAI/SUG2		161.3–301.1	54	nosp	99.86 melpt	C_{sat}	BSAO	65SUG/SEK
78BYV/JAS		293.1–333.1	3	2.00	not specified	C_p	BDCT	78BYV/JAS
79BRO/ZIE		159.0–306.0	eqn	nosp	99.94 melpt	C_p	BSAO	45SCO/MEY
82BEN/DAR		288.1–308.1	2	0.30	not specified	C_p	FSIT	71PIC/LED
82VIL/CAS		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
84STE/OLS		266.1–318.1	11S	nosp	not specified	C_p	BDHT	69PER/COM
84ZEG/SOM2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
85OGA		298.1	1	0.20	not specified	C_p	FSIO	85OGA
86KOR/KUK		298.0	1	0.20	not specified	C_p	BSAO	83KUK/KOR
86OGA/MUR		298.1	1	0.10	not specified	C_p	FSIO	85OGA
86TAN/TOY		298.1	1	0.30	99.96 anal	C_p	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FSIT	71PIC/LED
89PET/PES	N	258.1–318.1	4	0.20	not specified	C_p	BSAO	83KUK/KOR

25PAR same data in 27PAR/HUF
31FIO/GIN data calculated using procedure by 85WIL/CHA
60SWI/ZIE average value in temperature range 294–339 K
68PAZ/REC same datum in 70PAZ/PAZ
89PET/PES same data in 90ALP/PES

TABLE 42.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31FIO/GIN	318.1–378.1	7	0.20#	1.080	3.77–2	0.22	–1.50–2	–4
66HWA/ZIE	165.3–304.2	41	0.10#	0.431	5.60–3	0.04	1.87–3	13
66KLE	293.1–343.1	11	0.10	2.074	2.90–2	0.21	–1.31–2	–4
68PAZ/REC	313.1	1	0.30#	0.196	8.40–3	0.06	–8.40–3	–1
76FOR/BEN1	298.1	1	0.30	0.584	2.36–2	0.18	–2.36–2	–1
76FOR/BEN2	298.1	1	0.30	0.147	5.97–3	0.04	5.97–3	1
77HAI/SUG2	163.1–301.1	53	0.10#	0.716	8.65–3	0.07	2.24–3	5
79BRO/ZIE	159.0–305.7	10	0.20#	0.666	1.51–2	0.13	–1.37–2	–10
86OGA/MUR	298.1	1	0.10	0.620	8.37–3	0.06	8.37–3	1
89PET/PES	258.1–318.1	4	0.20	0.300	8.31–3	0.06	6.23–3	3
				Rejected data				
07WAL	(1.69–1, 1.26, 1.69–1, 1)			20GIB/PAR	(1.60–1, 1.50,–1.32–1, –9)			
24WIL/DAN	(4.74–1, 3.01, 3.81–1, 3)			25PAR	(7.26–2, 0.54, 4.78–2, 3)			
29KEL2	(8.13–2, 0.72,–5.67–2, –16)			29MIT/HAR1	(5.35–1, 4.46, 5.15–1, 25)			
31BLA/LEI	(7.79–1, 4.74, 6.94–1, 9)			36ERN/WAT	(1.08, 8.69,–1.08, –1)			
39BYK	(5.94–2, 0.44,–5.94–2, –1)			49TSC/RIC2	(4.51–1, 3.23, 4.51–1, 1)			
60SWI/ZIE	(1.47–1, 1.03,–1.47–1, –1)			62RAB/NIK	(8.45–2, 0.60, 3.35–2, 3)			
65KAU/BIT	(1.50–1, 1.07, 1.30–2, 5)			67GRA	(8.70–2, 0.60,–5.16–2, –4)			
67NIK/RAB2	(6.76–2, 0.64,–6.06–2, –19)			75PED/KAY	(2.32–1, 1.48, 1.96–1, 14)			
78BYV/JAS	(6.22–1, 4.34,–3.38–1, –1)			82BEN/DAR	(1.21–1, 0.86, 5.13–2, 0)			
82VIL/CAS	(1.76–1, 1.28, 1.76–1, 1)			84STE/OLS	(3.98–1, 2.85, 3.89–1, 11)			
84ZEG/SOM2	(4.57–2, 0.34, 4.57–2, 1)			85OGA	(2.14–1, 1.61,–2.14–1, –1)			
86KOR/KUK	(6.84–2, 0.50, 6.84–2, 1)			86TAN/TOY	(4.69–2, 0.35, 4.69–2, 1)			
88AND/PAT	(9.14–2, 0.68,–9.14–2, –1)							

TABLE 42.5.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	294	130	0.879	1.50–2	0.11	–1.41–3	3
C_{sat}	294	130	0.878	1.49–2	0.11	–1.40–3	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
159.0–220.0	1.09255+1	1.00327–1	–7.39674–1	3.32261–1	I
220.0–290.0	9.80631	1.62653	–1.43341	4.37372–1	I
290.0–378.2	2.50968+1	–1.41911+1	4.02096	–1.89566–1	II
159.0–220.0	1.08879+1	1.57505–1	–7.68386–1	3.37022–1	I
220.0–290.0	9.85835	1.56147	–1.40655	4.33714–1	I
290.0–378.2	2.63976+1	–1.55481+1	4.49332	–2.44431–1	II

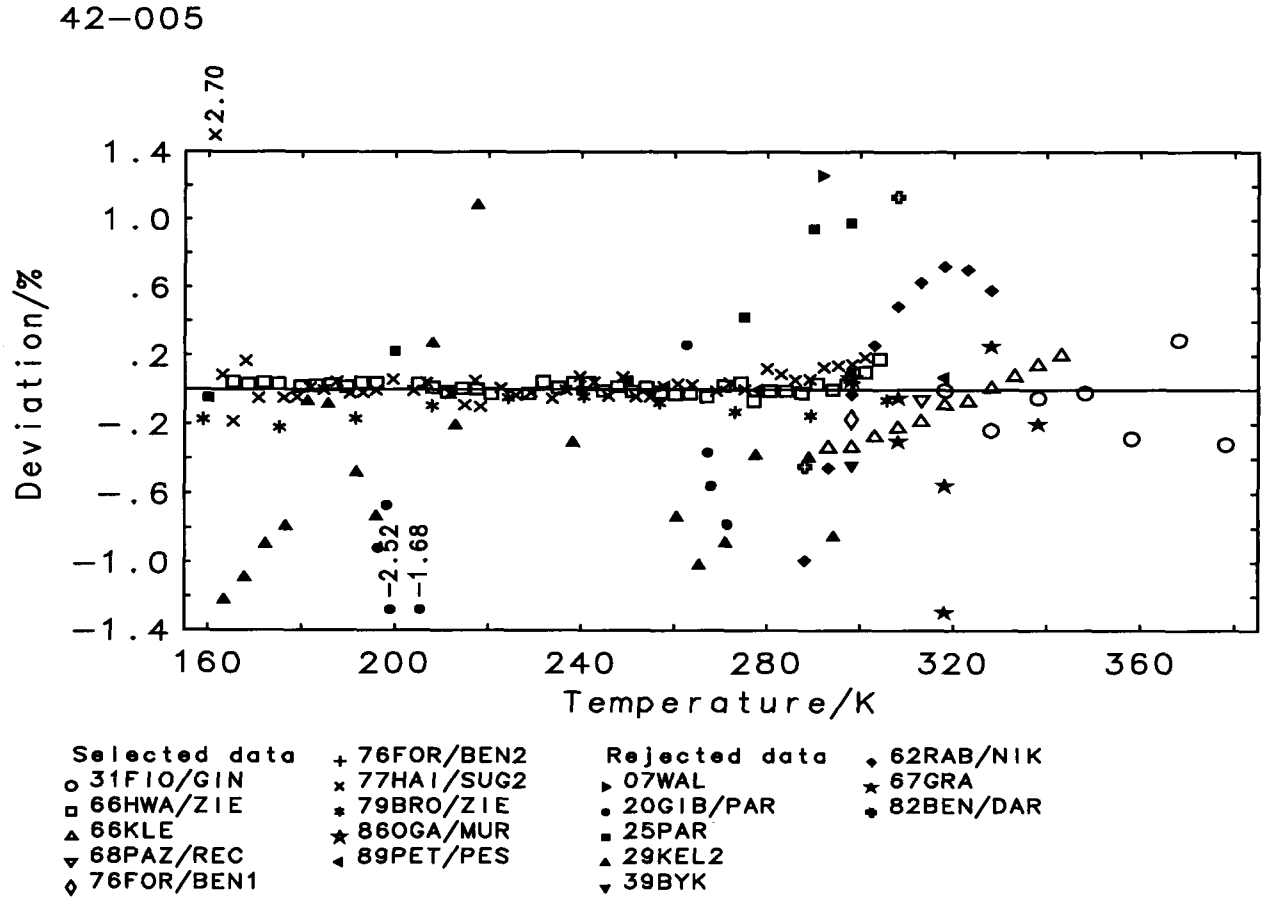
TABLE 42.5.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p ($J\,K^{-1}g^{-1}$)	1.9047	1.9114	1.9216	1.9356	1.9538	1.9765	2.0041
C_p ($J\,K^{-1}mol^{-1}$)	87.746	88.057	88.527	89.172	90.009	91.055	92.325
c_{sat} ($J\,K^{-1}g^{-1}$)	1.9047	1.9114	1.9216	1.9356	1.9538	1.9765	2.0041
C_{sat} ($J\,K^{-1}mol^{-1}$)	87.745	88.058	88.528	89.173	90.009	91.054	92.325
Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	2.0369	2.0755	2.1202	2.1717	2.2302	2.2502	2.2964
C_p ($J\,K^{-1}mol^{-1}$)	93.839	95.615	97.677	100.05	102.74	103.67	105.79
c_{sat} ($J\,K^{-1}g^{-1}$)	2.0369	2.0755	2.1202	2.1717	2.2302	2.2502	2.2964
C_{sat} ($J\,K^{-1}mol^{-1}$)	93.838	95.615	97.678	100.05	102.75	103.67	105.79
Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	2.3707	2.437	2.453	2.544	2.644	2.751	2.866
C_p ($J\,K^{-1}mol^{-1}$)	109.21	112.3	113.0	117.2	121.8	126.7	132.0
c_{sat} ($J\,K^{-1}g^{-1}$)	2.3707	2.437	2.453	2.544	2.643	2.750	2.864
C_{sat} ($J\,K^{-1}mol^{-1}$)	109.21	112.3	113.0	117.2	121.8	126.7	131.9
Temp. (K)	350	360	370	380			
c_p ($J\,K^{-1}g^{-1}$)	2.988	3.118	3.255	3.399			
C_p ($J\,K^{-1}mol^{-1}$)	137.7	143.6	149.9	156.6			
c_{sat} ($J\,K^{-1}g^{-1}$)	2.986	3.114	3.249	3.390			
C_{sat} ($J\,K^{-1}mol^{-1}$)	137.5	143.5	149.7	156.2			

TABLE 42.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	294	130	0.912	1.56–2	0.11	3.34–4	28

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
159.0–378.1	513.92	1.54028+1	3.59101–1	9.35649	2.57454+1	–4.14812+1	8.03298+1	II



Name: 1,2–Ethanediol
Formula: $C_2H_6O_2$

CAS–RN: 107–21–1
Group No.: 42–006
Molar Mass: 62.07

TABLE 42.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*98LOU	N	378.1–382.1	2	nosp	not specified		C_{avg}	DSIO	*98LOU
01DEF	N	309.4–349.1	2	nosp	not specified		C_{avg}	not specified	
02LOU1	N	380.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
09SCH		295.1–308.1	2	nosp	not specified		C_p	BSIO	09SCH
25PAR/KEL	N	262.0–293.0	6	nosp	99.	estim	C_p	BSIO	25PAR
32NEU/KUR		293.4–351.5	3	nosp	not specified		C_p	BSIO	32NEU
57CRU/JOS		293.1–338.1	2	2.00	not specified		C_p	BSIO	57CRU/JOS
62RAB/NIK		283.1–328.1	10S	0.30	not specified		C_p	BSAO	47SKU
65TUN/MIS		298.1	1	nosp	not specified		C_p	BSIO	49WEI
67NIK/RAB1		265.0–310.0	10S	nosp	not specified		C_p	BSAO	56POP/KOL
68PAZ/REC	N	301.1–313.1	2	nosp	not specified		C_p	BDCT	70PAZ/PAZ
72KAW/OTA		303.1	1	1.00	not specified		C_p	BSIO	49WEI
77MUR/SUB		298.1	1	0.30	not specified		C_p	BSIO	64MOE/THO
79STE/TAM		273.1–493.1	15S	nosp	99.9	chrom	C_{sat}	BDHT	69PER/COM
91DOU/PAL		298.1	1	nosp	99.5	estim	C_p	FSIT	71PIC/LED

*98LOU average values in temperature ranges 295–461 K and 296–468 K
01DEF average values in temperature ranges 286–412 K and 286–333 K; calorimeter not identified, probably drop
02LOU1 average value in temperature range 293–468 K
25PAR/KEL original values decreased by 1.5 %– correction for water content, recommendation given in 85WIL/CHA
68PAZ/REC same data in 70PAZ/PAZ

TABLE 42.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
25PAR/KEL	262.0–293.0	6	1.00#	0.493	8.41–2	0.49	–7.72–2	–6
62RAB/NIK	283.1–328.1	10	0.30	1.117	6.17–2	0.34	–2.94–2	–6
67NIK/RAB1	265.0–310.0	10	0.50#	1.140	1.03–1	0.57	9.01–2	10
68PAZ/REC	301.1	1	0.30#	0.293	1.59–2	0.09	1.59–2	1
77MUR/SUB	298.1	1	0.30	0.239	1.29–2	0.07	1.29–2	1
79STE/TAM	273.1–493.1	15	1.00#	0.115	2.41–2	0.12	–6.45–3	1
				Rejected data				
*98LOU	(4.15–1, 2.02,–4.15–1, –2)			01DEF	(2.45–1, 1.27,–2.30–1, –2)			
02LOU1	(2.34–1, 1.10, 2.34–1, 1)			09SCH	(1.69–1, 0.95,–5.98–2, 0)			
32NEU/KUR	(3.45–1, 1.84,–3.37–1, –3)			57CRU/JOS	(4.91, 18.59, 3.33, 0)			
65TUN/MIS	(2.70–1, 1.53,–2.70–1, –1)			72KAW/OTA	(7.17–1, 4.11, –7.17–1, –1)			
91DOU/PAL	(2.41–1, 1.36,–2.41–1, –1)							

TABLE 42.6.3. Parameters of regression polynomial

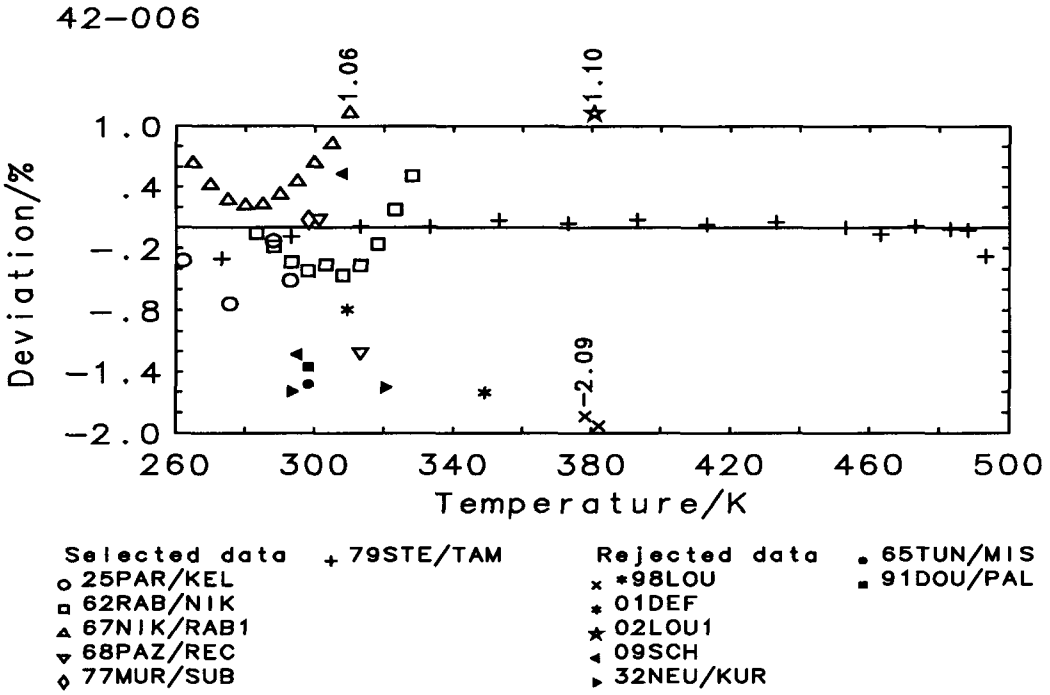
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	59	43	0.826	7.00–2	0.39	1.76–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
262.0–493.1		5.08850	4.81464	–1.64644–1			III

TABLE 42.6.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.262	2.279	2.315	2.367	2.409	2.418	2.469
C_p (J K^{-1}mol^{-1})	140.4	141.4	143.7	146.9	149.5	150.1	153.3
Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.520	2.570	2.620	2.669	2.718	2.766	2.814
C_p (J K^{-1}mol^{-1})	156.4	159.5	162.6	165.6	168.7	171.7	174.7
Temp. (K)	390	400	410	420	430	440	450
c_p (J K^{-1}g^{-1})	2.862	2.909	2.955	3.001	3.047	3.092	3.137
C_p (J K^{-1}mol^{-1})	177.6	180.5	183.4	186.3	189.1	191.9	194.7
Temp. (K)	460	470	480	490			
c_p (J K^{-1}g^{-1})	3.182	3.226	3.269	3.312			
C_p (J K^{-1}mol^{-1})	197.5	200.2	202.9	205.6			

TABLE 42.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	59	43	0.853	7.16–2	0.40	9.98–3	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
262.0–493.1	790.00	1.04312+1	5.87173–1	4.48624	4.63275+1		III



Name: 1,2,3–Propanetriol–*O*,*O*,*O*–d_3
Formula: $C_3H_5D_3O_3$

CAS–RN: 7325–16–8
Group No.: 42–007
Molar Mass: 95.11

TABLE 42.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62RAB/NIK	N	283.1–328.1	10S	0.30	not specified		C_p	BSAO	47SKU

62RAB/NIK sample deuterated to 97–98 mol.%

TABLE 42.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.030	2.49–3	0.01	–1.91–7	0
Temp. range K		A_1	A_2				Level of uncertainty
283.1–328.1		6.71136	7.06793				IV

TABLE 42.7.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	2.317	2.378	2.429	2.440	2.502	2.564	2.626
C_p ($J K^{-1} mol^{-1}$)	220.3	226.2	231.0	232.1	238.0	243.9	249.7

Name: 2–Propen–1–ol
Formula: C_3H_6O

CAS–RN: 107–18–6
Group No.: 42–008
Molar Mass: 58.08

TABLE 42.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		303.7–331.0	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*98LOU	N	331.1	1	nosp	not specified		C_{avg}	DSIO	*98LOU

*98LOU average value in temperature range 294–369 K

TABLE 42.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	303.7–331.0	4	3.00#	0.002	1.00–3	0.01	–9.54–7	0

TABLE 42.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	4	0.003	1.41–3	0.01	–9.54–7	0

Temp. range K	A_1	A_2	Level of uncertainty
303.7–331.0	4.41432–1	5.66447	V

TABLE 42.8.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c ($J K^{-1} g^{-1}$)	2.50	2.58	2.66	2.74
C ($J K^{-1} mol^{-1}$)	145	150	154	159

Name: 1–Propanol
Formula: C_3H_8O

CAS–RN: 71–23–8
Group No.: 42–009
Molar Mass: 60.10

TABLE 42.9.1. *Experimental heat capacities*

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
20GIB/PAR		165.7–274.6	29	nosp	not specified	C_p	BSIO	20GIB/LAT
26PAR/HUF	N	152.1–275.0	7	nosp	not specified	C_p	BSIO	25PAR
27PAR/HUF		169.1–275.3	7	nosp	not specified	C_p	BSIO	25PAR
29MIT/HAR1		162.8–274.4	35	nosp	not specified	C_p	BSIO	29MIT/HAR1
39PHI		301.1	1	nosp	not specified	C_p	BSIO	49WEI
41ZHD		279.6–318.8	5	nosp	not specified	C_p	BSIT	34KOL/UDO2
49TSC/RIC2		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
51EUC/EIG		273.0–393.0	12S	nosp	not specified	C_{sat}	BSAO	51EUC/EIG
60SWI/ZIE	N	320.9	1	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
68COU/LEE		153.9–361.5	47	0.10	99.75 melpt	C_p	BSAO	63AND/COU1
68PAZ/REC	N	313.1	1	nosp	not specified	C_p	BDCT	70PAZ/PAZ
68REC1	N	298.0–313.0	eqn	nosp	not specified	C_p	BSAO	68REC1
76FOR/BEN1		298.1–298.1	2	0.30	not specified	C_p	FSIT	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
77MUR/SUB		298.1	1	0.30	not specified	C_p	BSIO	64MOE/THO
79GRI/YAN	N	303.4–463.0	11	0.90	not specified	C_p	BDAO	75RAS/GRI
80KAL/JED		181.8–303.1	66	0.20	99.95 chrom	C_p	BSAO	80KAL/JED
81ARU/BAG		293.1–353.1	4S	1.50	99.0 melpt	C_p	BDHT	81ARU
82BEN/DAR		288.1–308.1	2S	0.30	not specified	C_p	FSIT	71PIC/LED
82VIL/CAS		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
84ZEG/SOM2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified	C_p	BSAO	83KUK/KOR
86TAN/TOY		298.1	1	0.30	99.9 anal	C_p	FSIT	71PIC/LED
91OGA/MIT		298.1	1	nosp	not specified	C_p	FSIO	85OGA

26PAR/HUF high sample purity
60SWI/ZIE average value in temperature range 294–347 K
68PAZ/REC same datum in 70PAZ/PAZ
68REC1 same data in 68REC2 and 68REC3
79GRI/YAN data above 343.28 K measured at elevated pressures up to 1.52 MPa

TABLE 42.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68COU/LEE	153.9–361.5	47	0.10	1.217	2.17–2	0.12	2.14–3	1
76FOR/BEN1	298.1	2	0.30	0.363	1.89–2	0.11	1.72–2	2
76FOR/BEN2	298.1	1	0.30	0.036	1.86–3	0.01	1.86–3	1
79GRI/YAN	303.4–463.0	11	0.90	0.870	2.16–1	0.78	–4.17–2	–5
80KAL/JED	181.8–303.1	64	0.20	0.613	1.81–2	0.12	–5.90–3	–16
86TAN/TOY	298.1	1	0.30	0.244	1.27–2	0.07	1.27–2	1
91OGA/MIT	298.1	1	0.30#	0.475	2.46–2	0.14	–2.46–2	–1
				Rejected data				
20GIB/PAR	(1.03–1, 0.74, 2.14–2, 7)			26PAR/HUF	(1.26–1, 0.83, 1.17–1, 5)			
27PAR/HUF	(1.21–1, 0.84, 1.17–1, 7)			29MIT/HAR1	(7.89–1, 5.22, 7.30–1, 31)			
39PHI	(2.30, 11.61, 2.30, 1)			41ZHD	(4.09–1, 2.17, 3.50–1, 5)			
49TSC/RIC2	(5.71–1, 3.19, 5.71–1, 1)			51EUC/EIG	(4.61–1, 2.50, –4.01–1, –10)			
60SWI/ZIE	(2.85–1, 1.52,–2.85–1, –1)			68PAZ/REC	(6.96–1, 3.65, 6.96–1, 1)			
68REC1	(1.80–1, 1.02, 5.00–2, 0)			77MUR/SUB	(6.19–1, 3.45, 6.19–1, 1)			
81ARU/BAG	(2.76–1, 1.39,–2.13–1, –2)			82BEN/DAR	(1.85–1, 1.01, 1.28–1, 0)			
82VIL/CAS	(3.64–1, 2.06, 3.64–1, 1)			84ZEG/SOM2	(7.04–2, 0.41, 7.04–2, 1)			
86KOR/KUK	(8.81–2, 0.52, 8.72–2, 2)							

TABLE 42.9.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	243	127	0.921	6.78–2	0.26	–5.60–3	–17
C_{sat}	243	127	0.923	6.28–2	0.25	–5.31–3	–16

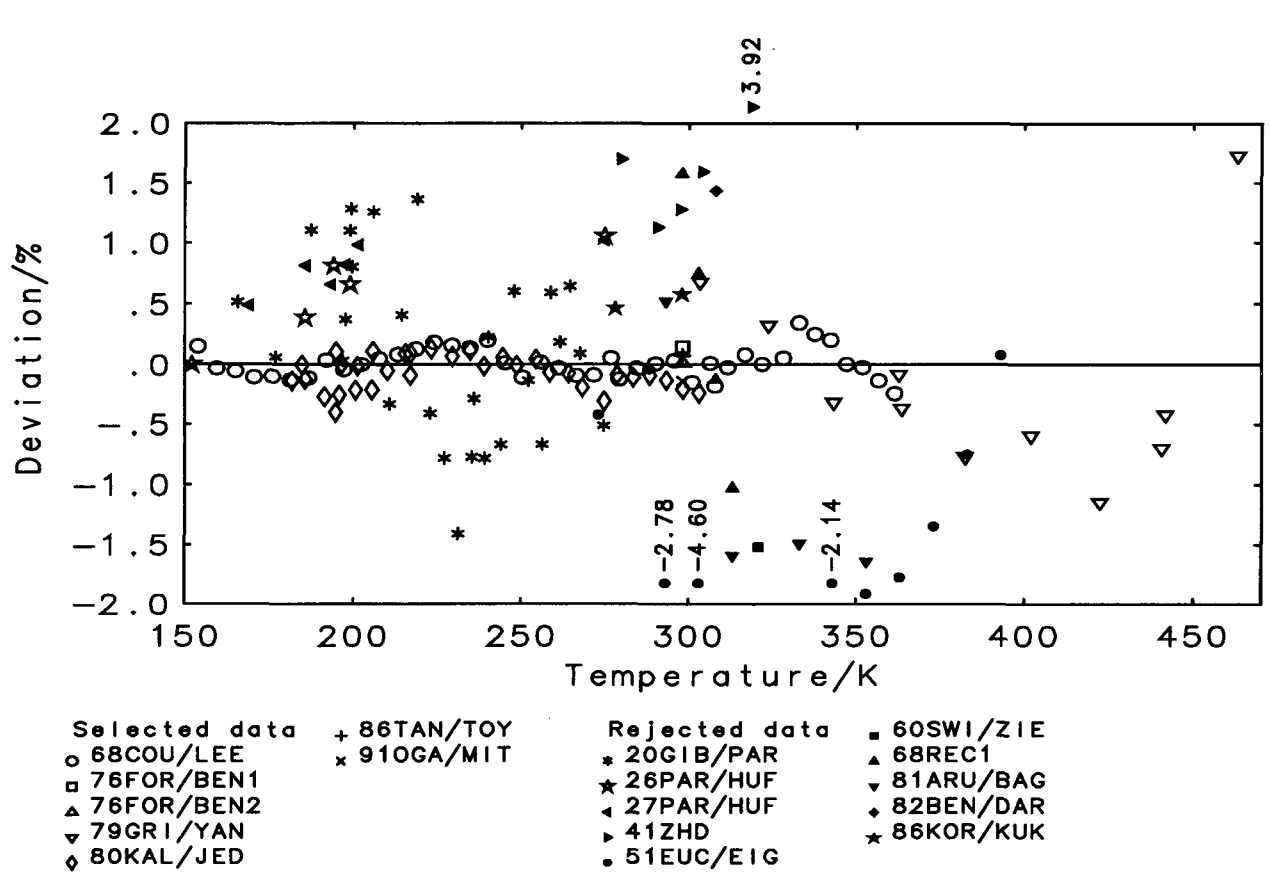
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
153.9–260.0	9.59808	5.25961	–3.31637	8.13095–1	II
260.0–330.0	2.46638+1	–1.21239+1	3.36958	–4.40775–2	II
330.0–463.0	1.33502+2	–1.11068+2	3.33525+1	–3.07266	IV
153.9–260.0	9.56721	5.30528	–3.33846	8.16591–1	II
260.0–330.0	2.49853+1	–1.24849+1	3.50391	–6.06356–2	II
330.0–463.0	1.38348+2	–1.15542+2	3.47334+1	–3.21513	IV

TABLE 42.9.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.767	1.778	1.792	1.807	1.826	1.848	1.874
C_p (J K^{-1}mol^{-1})	106.2	106.9	107.7	108.6	109.7	111.1	112.6
c_{sat} (J K^{-1}g^{-1})	1.767	1.778	1.792	1.807	1.826	1.848	1.874
C_{sat} (J K^{-1}mol^{-1})	106.2	106.9	107.7	108.6	109.7	111.1	112.6
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.906	1.943	1.987	2.037	2.095	2.162	2.185
C_p (J K^{-1}mol^{-1})	114.5	116.8	119.4	122.4	125.9	129.9	131.3
c_{sat} (J K^{-1}g^{-1})	1.906	1.943	1.987	2.037	2.095	2.162	2.185
C_{sat} (J K^{-1}mol^{-1})	114.5	116.8	119.4	122.4	125.9	129.9	131.3
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.237	2.320	2.394	2.411	2.511	2.619	2.735
C_p (J K^{-1}mol^{-1})	134.4	139.4	143.9	144.9	150.9	157.4	164.3
c_{sat} (J K^{-1}g^{-1})	2.237	2.320	2.394	2.411	2.511	2.619	2.734
C_{sat} (J K^{-1}mol^{-1})	134.4	139.4	143.9	144.9	150.9	157.4	164.3
Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	2.858	2.988	3.120	3.253	3.383	3.509	3.628
C_p (J K^{-1}mol^{-1})	171.8	179.5	187.5	195.5	203.3	210.9	218.0
c_{sat} (J K^{-1}g^{-1})	2.858	2.987	3.118	3.249	3.378	3.502	3.617
C_{sat} (J K^{-1}mol^{-1})	171.7	179.5	187.4	195.3	203.0	210.4	217.4
Temp. (K)	410	420	430	440	450	460	
c_p (J K^{-1}g^{-1})	3.737	3.834	3.916	3.980	4.025	4.047	
C_p (J K^{-1}mol^{-1})	224.6	230.4	235.3	239.2	241.9	243.2	
c_{sat} (J K^{-1}g^{-1})	3.722	3.814	3.889	3.946	3.982	3.994	
C_{sat} (J K^{-1}mol^{-1})	223.7	229.2	233.7	237.2	239.3	240.0	

TABLE 42.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	243	127	2.195	7.03–2	0.34	2.00–3	7
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
153.9–463.0	536.78	1.04907+2	5.51787	5.64004	1.22718+2	–6.15566+1	2.05196+2	IV



Name: 2–Propanol
Formula: C_3H_8O

CAS–RN: 67–63–0
Group No.: 42–010
Molar Mass: 60.10

TABLE 42.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
24WIL/DAN		303.0–328.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
25PAR/KEL		195.4–293.1	9	nosp	not specified	C_p	BSIO	25PAR
28PAR/KEL	N	195.4–293.1	11	1.00	99.96 estim	C_p	BSIO	25PAR
29KEL3		188.4–292.8	12	1.00	99.95 estim	C_p	BSIO	29KEL1
33TRE/WAT		298.1	1	nosp	not specified	C_p	BSIO	49WEI
39PHI		303.1	1	nosp	not specified	C_p	BSIO	49WEI
45ZHD		280.0–320.0	4	nosp	not specified	C_p	BSIT	34KOL/UDO2
48GIN/COR		273.1–473.1	11S	nosp	not specified	C_{sat}	DSTO	50GIN/DOU
58SWI/ZIE2	N	324.0	1	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
62KAT		293.1–343.1	3	nosp	not specified	C_p	BSIO	62KAT
63AND/COU2		188.3–327.1	60	nosp	not specified	C_p	BSAO	63AND/COU1
77HOF/SAN	N	353.1–463.1	12S	1.00	not specified	C_p	FSIO	75SAN
79BRO/ZIE		185.0–304.0	eqn	nosp	99.84 melpt	C_p	BSAO	45SCO/MEY
79GRI/YAN		329.3–341.5	2	0.90	not specified	C_p	BDAO	75RAS/GRI
80ROU/ROB		283.1–298.1	2	0.30	not specified	C_p	FSIT	71PIC/LED
86KOR/KUK		298.0	1	0.20	not specified	C_p	BSAO	83KUK/KOR

28PAR/KEL similar data in 25PAR/KEL
58SWI/ZIE2 average value in temperature range 294–354 K
77HOF/SAN C_p at saturation curve extrapolated from high pressure measurements

TABLE 42.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
48GIN/COR	273.1–473.1	11	0.80#	0.956	1.79–1	0.76	–6.31–2	–3
63AND/COU2	188.3–327.1	60	0.20#	1.216	4.56–2	0.24	2.97–3	–4
79BRO/ZIE	185.0–304.6	24	0.30#	0.752	3.56–2	0.23	–1.09–2	–4
79GRI/YAN	329.3–341.5	2	0.90	0.424	8.38–2	0.38	4.09–2	0
				Rejected data				
24WIL/DAN	(1.47, 6.71, 1.47, 3)			25PAR/KEL	(1.00–1, 0.65, 9.18–2, 7)			
28PAR/KEL	(7.43–2, 0.50, 2.34–2, 3)			29KEL3	(2.27–1, 1.50,–2.02–1, –12)			
33TRE/WAT	(9.96–1, 5.07, 9.96–1, 1)			39PHI	(1.61, 7.74, 1.61, 1)			
45ZHD	(6.72–1, 3.26, 6.12–1, 4)			58SWI/ZIE2	(4.74–1, 2.18, 4.74–1, 1)			
62KAT	(8.27–1, 4.00, 8.00–1, 3)			77HOF/SAN	(7.79–1, 2.73, 7.43–1, 12)			
80ROU/ROB	(5.28–1, 2.74, 4.49–1, 2)			86KOR/KUK	(1.04–1, 0.56, 1.04–1, 1)			

TABLE 42.10.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	157	97	1.113	7.56–2	0.36	–7.17–3	–11
C_{sat}	157	97	1.110	7.70–2	0.36	–7.79–3	–10

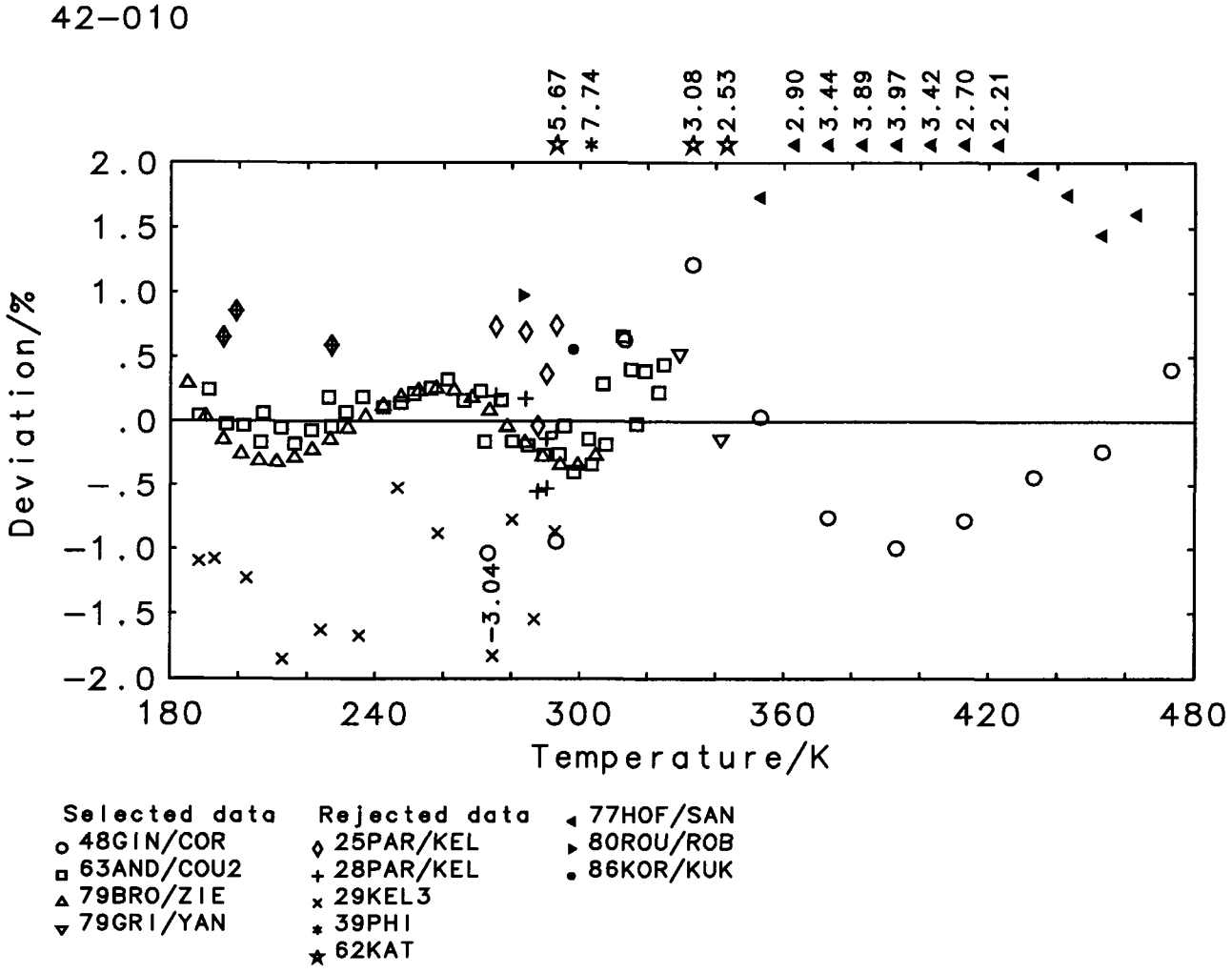
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
185.0–270.0	–1.07714+1	3.21323+1	–1.52462+1	2.61461	II
270.0–360.0	1.11378+2	–1.03589+2	3.50209+1	–3.59120	IV
360.0–473.2	–1.72015+2	1.32572+2	–3.05794+1	2.48290	V
185.0–270.0	–1.06348+1	3.19569+1	–1.51720+1	2.60430	II
270.0–360.0	1.11418+2	–1.03657+2	3.50554+1	–3.59663	IV
360.0–473.2	–1.23195+2	9.18532+1	–1.92531+1	1.43194	V

TABLE 42.10.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.823	1.857	1.893	1.933	1.977	2.030	2.092
C_p (J K^{-1}mol^{-1})	109.5	111.6	113.8	116.1	118.8	122.0	125.7
c_{sat} (J K^{-1}g^{-1})	1.823	1.857	1.893	1.933	1.977	2.030	2.092
C_{sat} (J K^{-1}mol^{-1})	109.5	111.6	113.8	116.1	118.8	122.0	125.8
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.167	2.256	2.287	2.360	2.478	2.582	2.606
C_p (J K^{-1}mol^{-1})	130.2	135.6	137.4	141.8	148.9	155.2	156.6
c_{sat} (J K^{-1}g^{-1})	2.167	2.256	2.287	2.360	2.478	2.582	2.606
C_{sat} (J K^{-1}mol^{-1})	130.2	135.6	137.4	141.8	148.9	155.1	156.6
Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.742	2.882	3.024	3.164	3.300	3.428	3.55
C_p (J K^{-1}mol^{-1})	164.8	173.2	181.7	190.1	198.3	206.0	213
c_{sat} (J K^{-1}g^{-1})	2.742	2.882	3.023	3.163	3.298	3.426	3.54
C_{sat} (J K^{-1}mol^{-1})	164.8	173.2	181.7	190.1	198.2	205.9	213
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	3.66	3.76	3.86	3.96	4.06	4.16	4.26
C_p (J K^{-1}mol^{-1})	220	226	232	238	244	250	256
c_{sat} (J K^{-1}g^{-1})	3.65	3.75	3.85	3.94	4.02	4.10	4.18
C_{sat} (J K^{-1}mol^{-1})	220	226	231	237	242	246	251
Temp. (K)	450	460	470				
c_p (J K^{-1}g^{-1})	4.37	4.49	4.62				
C_p (J K^{-1}mol^{-1})	263	270	277				
c_{sat} (J K^{-1}g^{-1})	4.26	4.33	4.41				
C_{sat} (J K^{-1}mol^{-1})	256	260	265				

TABLE 42.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	157	97	2.435	2.99–1	1.05	7.33–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
185.0–473.1	508.30	1.59868+2	9.16183	9.30500–2	1.94473+2	–1.07654+2	2.99943+2	V



Name: 1,2–Propanediol
Formula: $C_3H_8O_2$

CAS–RN: 57–55–6
Group No.: 42–011
Molar Mass: 76.10

TABLE 42.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
27PAR/HUF		194.3–276.6	7	nosp	not specified		C_p	BSIO	25PAR
52CUR/JOH	N	213.1–460.5	26S	nosp	not specified		C_{sat}	not specified	
72KAW/OTA		303.1	1	1.00	not specified		C_p	BSIO	49WEI

52CUR/JOH correlated data (sources: Dow Chemical Co.(technical product) and 27PAR/HUF)

TABLE 42.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
27PAR/HUF	194.3–276.6	7	1.00#	0.201	3.81–2	0.20	6.86–3	1
52CUR/JOH	213.1–460.5	26	3.00#	0.187	1.21–1	0.56	–1.52–2	0
				Rejected data				
72KAW/OTA	(1.55, 7.17,–1.55, –1)							

TABLE 42.11.3. Parameters of regression polynomial

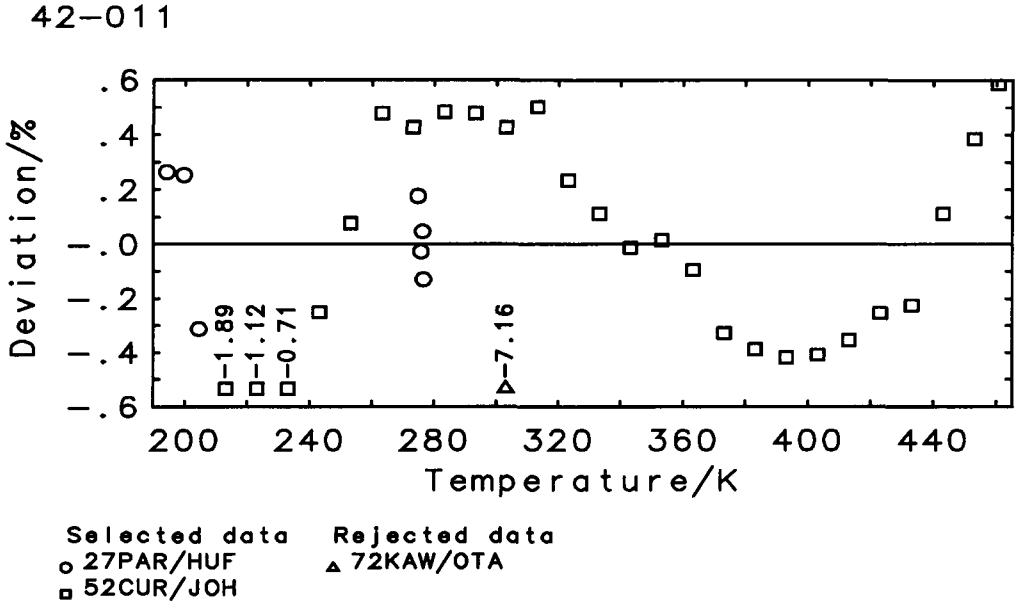
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	34	33	0.202	1.16–1	0.54	–1.05–2	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
194.3–460.5		2.04442+1	–7.01228	3.69315	–3.58297–1		V

TABLE 42.11.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c ($J\,K^{-1}g^{-1}$)	1.97	2.00	2.04	2.08	2.13	2.18	2.23
C ($J\,K^{-1}mol^{-1}$)	150	152	155	159	162	166	170
Temp. (K)	260	270	273.15	280	290	298.15	300
c ($J\,K^{-1}g^{-1}$)	2.28	2.34	2.35	2.39	2.45	2.50	2.51
C ($J\,K^{-1}mol^{-1}$)	174	178	179	182	186	190	191
Temp. (K)	310	320	330	340	350	360	370
c ($J\,K^{-1}g^{-1}$)	2.57	2.63	2.69	2.75	2.82	2.88	2.94
C ($J\,K^{-1}mol^{-1}$)	196	200	205	210	214	219	224
Temp. (K)	380	390	400	410	420	430	440
c ($J\,K^{-1}g^{-1}$)	3.00	3.06	3.12	3.18	3.23	3.29	3.34
C ($J\,K^{-1}mol^{-1}$)	228	233	237	242	246	250	254
Temp. (K)	450	460					
c ($J\,K^{-1}g^{-1}$)	3.39	3.44					
C ($J\,K^{-1}mol^{-1}$)	258	262					

TABLE 42.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C	34	33	0.431	2.33–1	0.95	5.46–2	1 0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
194.3–460.5	688.00	−7.55007	7.76903–1	9.16907	1.83432+1		V



Name: 1,2,3–Propanetriol
Formula: $C_3H_8O_3$

CAS–RN: 56–81–5
Group No.: 42–012
Molar Mass: 92.09

TABLE 42.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*79BER	N	330.1–380.6	3	nosp	not specified	C_{avg}	DSIO	*79BER
22SIM		294.4	1	nosp	not specified	C_p	BSIO	23SIM/LAN
23GIB/GIA		299.4	1	nosp	99.67 melpt	C_p	BSIO	20GIB/LAT
27PAR/HUF		299.4	1	nosp	not specified	C_p	BSIO	25PAR
36ERN/WAT		298.1	1	nosp	not specified	C_p	BSIO	49WEI
62OME1	N	293.1–453.1	6S	nosp	not specified	C_p	not specified	
62RAB/NIK		293.1–328.1	8S	0.30	not specified	C_p	BSAO	47SKU
68PAZ/REC	N	301.1–313.1	2	nosp	not specified	C_p	BDCT	70PAZ/PAZ
77MUR/SUB		298.1	1	0.30	not specified	C_p	BSIO	64MOE/THO
81ATA/ELS		293.1	1	2.50	not specified	C_p	BDHO	81ATA/ELS
88BAS/NIL		298.1	1	nosp	not specified	C_p	DDCT	74SUU/WAD

*79BER average values in temperature ranges 287–373 K, 289–452 K and 293–468 K
62OME1 the first 3 data pnts.from:Nevolin F.V.:Chim.i Tekhn.Proizv.Glicerina,1954;
Zozulya N.V.:Teploper.iTepl.Model.,ANSSSR 1959
68PAZ/REC same data in 70PAZ/PAZ

TABLE 42.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*79BER	330.1–380.6	3	3.00#	0.676	5.77–1	2.03	–5.46–1	–3
62OME1	293.1–353.1	4	3.00#	0.343	2.75–1	1.03	7.74–2	0
62RAB/NIK	293.1–328.1	8	0.30	0.448	3.69–2	0.13	–6.96–3	–2
88BAS/NIL	298.1	1	0.30#	0.900	7.11–2	0.27	7.11–2	1
				Rejected data				
22SIM	(9.23–1, 3.42, 9.23–1, 1)			23GIB/GIA	(5.26–1, 1.96, 5.26–1, 1)			
27PAR/HUF	(5.26–1, 1.96, 5.26–1, 1)			36ERN/WAT	(5.36–1, 2.08, –5.36–1, –1)			
68PAZ/REC	(2.08, 6.93, 1.58, 2)			77MUR/SUB	(4.32–1, 1.62, 4.32–1, 1)			
81ATA/ELS	(4.00–1, 1.52, 4.00–1, 1)							

TABLE 42.12.3. Parameters of regression polynomial

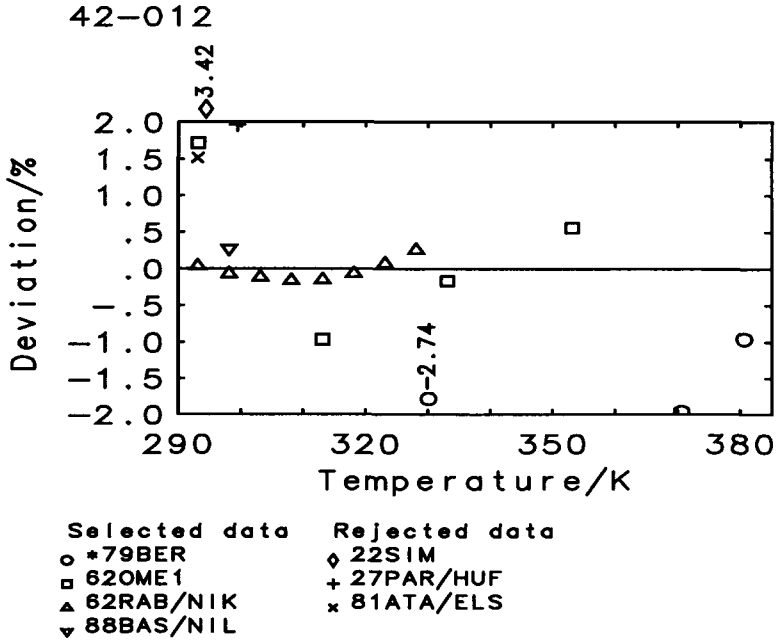
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	16	0.551	3.07–1	1.09	–8.20–2	–4
Temp. range K		A_1	A_2				Level of uncertainty
293.1–380.6		8.69757	5.88927				V

TABLE 42.12.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.38	2.43	2.49	2.54	2.59	2.65	2.70
C_p (J K^{-1}mol^{-1})	219	224	229	234	239	244	249
Temp. (K)	370	380					
c_p (J K^{-1}g^{-1})	2.75	2.81					
C_p (J K^{-1}mol^{-1})	253	258					

TABLE 42.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	16	0.838	2.69–1	0.97	1.95–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
293.1–380.6	800.00	1.19937+1	5.72867–1	7.52628	6.27762+1		V



Name: 1–Butanol
Formula: $C_4H_{10}O$

CAS–RN: 71–36–3
Group No.: 42–013
Molar Mass: 74.12

TABLE 42.13.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
24WIL/DAN		303.0–348.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
25PAR		194.6–294.0	12	0.50	not specified	C_p	BSIO	25PAR
33TRE/WAT		298.1	1	nosp	not specified	C_p	BSIO	49WEI
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified	C_p	not specified	
39PHI		302.5	1	nosp	not specified	C_p	BSIO	49WEI
49TSC/RIC2		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
60SWI/ZIE	N	322.4	1	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
65COU/HAL		188.2–322.3	25	0.20	99.94 melpt	C_p	BSAO	63AND/COU1
67GRA		308.1–338.1	4	1.00	not specified	C_p	BSIO	67GRA
68PAZ/REC	N	301.1–313.1	2	nosp	not specified	C_p	BDCT	70PAZ/PAZ
75SAN	N	295.9–466.6	20	0.90	not specified	C_p	FSIO	75SAN
78BYV/JAS		293.1–333.1	3	2.00	not specified	C_p	BDCT	78BYV/JAS
79GRI/YAN	N	324.0–462.5	8S	0.90	not specified	C_p	BDAO	75RAS/GRI
81ARU/BAG		293.1–373.1	5S	1.50	not specified	C_p	BDHT	81ARU
86GAT/WOO		298.1–368.1	4	nosp	99. anal	C_p	BDCT	83ROU/ROU
86KOR/KUK		278.0–298.0	2	0.20	not specified	C_p	BSAO	83KUK/KOR
86NAZ/BAS1		321.0–373.4	3	2.00	not specified	C_p	BDHO	86NAZ/BAS1
86OGA/MUR		298.1	1	0.10	not specified	C_p	FSIO	85OGA
86ROU/GRO		298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
86TAN/TOY		298.1	1	0.30	99.9 anal	C_p	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FSIT	71PIC/LED
88PIE/SOM2		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	99.5 anal	C_p	FSIT	71PIC/LED

38PAN/DUD temperature range of parameters validity estimated by the compilers
60SWI/ZIE average value in temperature range 294–350 K
68PAZ/REC same data in 70PAZ/PAZ; apparently wrong value at 313.15 K
75SAN C_p at pressure near 1.4 MPa
79GRI/YAN data above 363.61 K measured at elevated pressures up to 0.92 MPa

TABLE 42.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65COU/HAL	188.2–322.3	25	0.20	0.961	4.08–2	0.19	4.38–3	0
68PAZ/REC	301.1	1	0.50#	0.385	4.16–2	0.19	4.16–2	1
75SAN	295.9–466.6	19	0.90	0.995	2.54–1	0.90	–4.39–2	–3
79GRI/YAN	324.0–462.5	8	0.90	1.011	2.97–1	0.91	1.08–1	–2
86GAT/WOO	298.1–368.1	4	0.40#	0.973	1.01–1	0.39	–9.63–2	–4
86OGA/MUR	298.1	1	0.10	0.324	6.91–3	0.03	6.91–3	1
86TAN/TOY	298.1	1	0.30	0.816	5.20–2	0.24	–5.20–2	–1
88AND/PAT	298.1	1	0.30#	0.495	3.16–2	0.15	–3.16–2	–1
88PIE/SOM2	298.1	1	0.30#	0.080	5.11–3	0.02	–5.11–3	–1
				Rejected data				
24WIL/DAN	(8.27–2, 0.35, 2.69–2, 2)			25PAR	(7.86–2, 0.39, 2.78–2, 4)			
33TRE/WAT	(7.41–1, 3.36, 7.41–1, 1)			38PAN/DUD	(1.38, 5.72, 1.05, 3)			
39PHI	(4.25, 16.39, 4.25, 1)			49TSC/RIC2	(8.91–1, 4.01, 8.91–1, 1)			
60SWI/ZIE	(7.99–1, 3.51,–7.99–1, –1)			67GRA	(2.68–1, 1.14,–2.38–1, –4)			
78BYV/JAS	(2.14, 10.05, –1.83, –3)			81ARU/BAG	(4.20–1, 1.64,–3.57–1, –3)			
86KOR/KUK	(9.93–2, 0.49, 9.80–2, 2)			86NAZ/BAS1	(9.66–1, 3.65, –8.71–1, –3)			
86ROU/GRO	(1.39–1, 0.65,–1.39–1, –1)			89COB/GAR	(2.38–1, 1.13, –2.38–1, –1)			

TABLE 42.13.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	107	61	1.001	1.92–1	0.65	–4.68–3	–10
C_{sat}	107	61	1.002	1.92–1	0.66	–4.78–3	–10

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
188.2–310.0	1.51439+1	2.17621	–2.15182	7.09291–1	II
310.0–390.0	1.79072+2	–1.56464+2	4.90224+1	–4.79332	IV
390.0–466.6	–3.86930+2	2.78922+2	–6.26150+1	4.74835	V
188.2–310.0	1.51536+1	2.16438	–2.14706	7.08663–1	II
310.0–390.0	1.80381+2	–1.57733+2	4.94327+1	–4.83754	IV
390.0–466.6	–3.72390+2	2.67475+2	–5.95950+1	4.48106	V

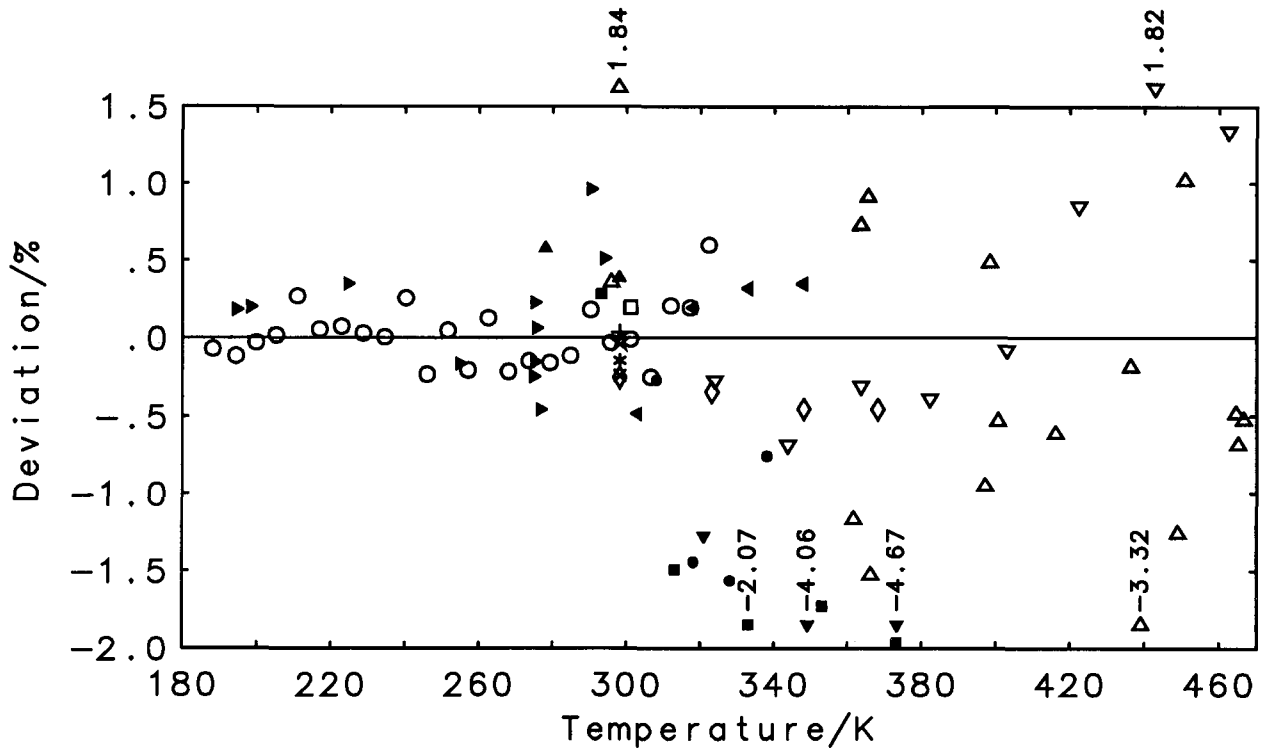
TABLE 42.13.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	1.837	1.858	1.884	1.915	1.951	1.994	2.044
C_p ($J\,K^{-1}mol^{-1}$)	136.2	137.7	139.6	141.9	144.6	147.8	151.5
c_{sat} ($J\,K^{-1}g^{-1}$)	1.837	1.858	1.884	1.915	1.951	1.994	2.044
C_{sat} ($J\,K^{-1}mol^{-1}$)	136.2	137.7	139.6	141.9	144.6	147.8	151.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.100	2.164	2.186	2.236	2.317	2.390	2.407
C_p ($J\,K^{-1}mol^{-1}$)	155.7	160.4	162.0	165.8	171.8	177.1	178.4
c_{sat} ($J\,K^{-1}g^{-1}$)	2.100	2.164	2.186	2.236	2.317	2.390	2.407
C_{sat} ($J\,K^{-1}mol^{-1}$)	155.7	160.4	162.0	165.8	171.8	177.1	178.4
Temp. (K)	310	320	330	340	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	2.506	2.615	2.730	2.849	2.968	3.084	3.194
C_p ($J\,K^{-1}mol^{-1}$)	185.8	193.8	202.4	211.2	220.0	228.6	236.8
c_{sat} ($J\,K^{-1}g^{-1}$)	2.506	2.615	2.730	2.849	2.968	3.084	3.193
C_{sat} ($J\,K^{-1}mol^{-1}$)	185.8	193.8	202.4	211.2	220.0	228.6	236.7
Temp. (K)	380	390	400	410	420	430	440
c_p ($J\,K^{-1}g^{-1}$)	3.295	3.383	3.46	3.52	3.57	3.61	3.65
C_p ($J\,K^{-1}mol^{-1}$)	244.2	250.8	256	261	264	268	271
c_{sat} ($J\,K^{-1}g^{-1}$)	3.293	3.380	3.45	3.51	3.56	3.60	3.64
C_{sat} ($J\,K^{-1}mol^{-1}$)	244.1	250.6	256	260	264	267	270
Temp. (K)	450	460	470				
c_p ($J\,K^{-1}g^{-1}$)	3.70	3.74	3.79				
C_p ($J\,K^{-1}mol^{-1}$)	274	277	281				
c_{sat} ($J\,K^{-1}g^{-1}$)	3.68	3.72	3.76				
C_{sat} ($J\,K^{-1}mol^{-1}$)	273	275	279				

TABLE 42.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	107	61	1.975	3.20–1	1.10	3.85–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
188.2–466.6	563.05	2.49634+2	1.68946+1	–3.13552	2.64765+2	–4.94325+1	3.39538+2	V

42–013



Selected data
- 65COU/HAL
- 68PAZ/REC
- 75SAN
- 79GRI/YAN
- 86GAT/WOO
- 86OGA/MUR
- 86TAN/TOY
- 88AND/PAT
- 88PIE/SOM2

Rejected data
- 24WIL/DAN
- 25PAR
- 67GRA
- 81ARU/BAG
- 86KOR/KUK
- 86NAZ/BAS1

Name: 2-Butanol
Formula: $C_4H_{10}O$

CAS-RN: 78-92-2
Group No.: 42-014
Molar Mass: 74.12

TABLE 42.14.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified	C_p	not specified	
76CON/GIA		298.1	1	nosp	not specified	C_p	BDCT	76CON/GIA
88OKA/OGA	N	298.1	1	nosp	not specified	C_p	FSIO	85OGA

38PAN/DUD temperature range of parameters validity estimated by the compilers
88OKA/OGA water content below 0.083 mol.%

Name: (*R*,*S*)–2–Butanol
Formula: $C_4H_{10}O$

CAS–RN: 15892–23–6
Group No.: 42–015
Molar Mass: 74.12

TABLE 42.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36PAR/THO	276.5–281.7	3	1.00	not specified		C_p	BSIO	25PAR
71AND/CON	188.4–345.5	61	nosp	99.95	melpt	C_p	BSAO	63AND/COU1
88PIE/SOM1	298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED

TABLE 42.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71AND/CON	188.4–345.5	61	0.20#	0.410	1.65–2	0.08	7.94–6	1
				Rejected data				
36PAR/THO	(4.56–1, 2.08, 4.47–1, 3)			88PIE/SOM1	(1.74–2, 0.07, –1.74–2, –1)			

TABLE 42.15.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	61	0.427	1.72–2	0.09	7.94–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
188.4–280.0		1.00923+1	9.26705	–6.26981	1.57517		II
280.0–345.4		2.44274+2	–2.41642+2	8.33405+1	–9.09272		II

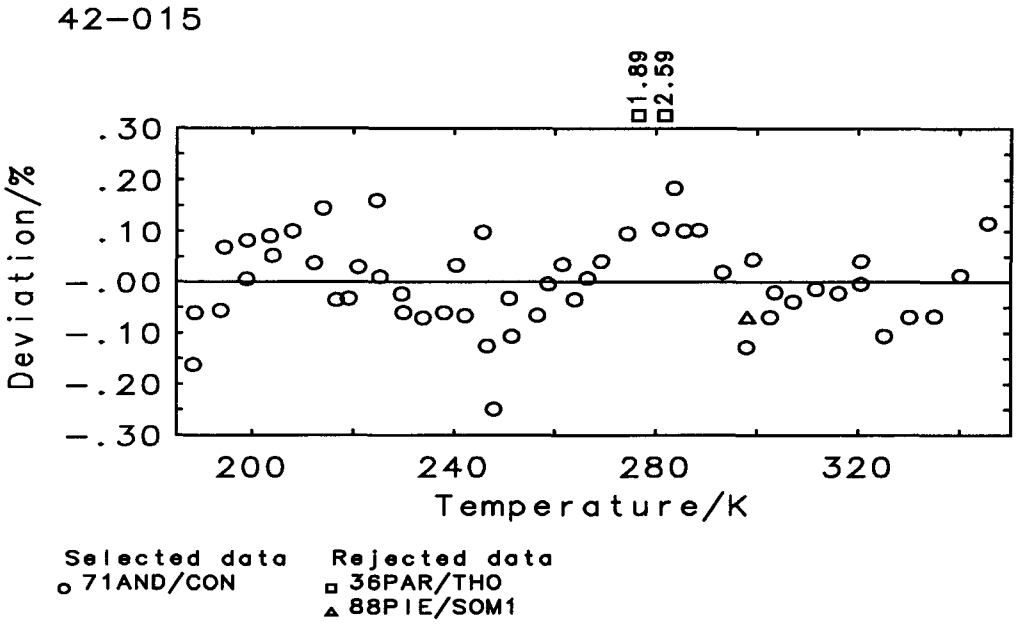
TABLE 42.15.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	1.780	1.811	1.850	1.896	1.952	2.018	2.096
C_p ($J\,K^{-1}mol^{-1}$)	131.9	134.3	137.1	140.6	144.7	149.6	155.4
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	2.186	2.289	2.325	2.408	2.540	2.655	2.682
C_p ($J\,K^{-1}mol^{-1}$)	162.0	169.7	172.3	178.5	188.3	196.8	198.8
Temp. (K)	310	320	330	340	350		
c_p ($J\,K^{-1}g^{-1}$)	2.827	2.970	3.104	3.222	3.3201		
C_p ($J\,K^{-1}mol^{-1}$)	209.6	220.1	230.1	238.9	246.09		

TABLE 42.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	61	1.532	6.44–2	0.31	5.21–4	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
188.4–345.5	536.05	1.20927+3	1.06657+2	–1.05987+2	1.27296+3	–1.66913+2	1.25135+3	III



Name: (*S*)–2–Butanol
Formula: $C_4H_{10}O$

CAS–RN: 4221–99–2
Group No.: 42–016
Molar Mass: 74.12

TABLE 42.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71AND/CON	180.1–309.7	35	nosp	99.85	melpt	C_p	BSAO	63AND/COU1

TABLE 42.16.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	35	35	0.337	1.47–2	0.07	1.86–5	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
180.1–250.0	–7.87841–1	2.43906+1	–1.32324+1	2.63606	II
250.0–309.7	6.24594+1	–5.15060+1	1.71263+1	–1.41176	II

TABLE 42.16.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.752	1.780	1.812	1.850	1.895	1.950	2.016
C_p (J K^{-1}mol^{-1})	129.8	131.9	134.3	137.1	140.5	144.5	149.4
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.095	2.188	2.295	2.331	2.414	2.545	2.661
C_p (J K^{-1}mol^{-1})	155.3	162.2	170.1	172.8	178.9	188.7	197.2
Temp. (K)	300	310					
c_p (J K^{-1}g^{-1})	2.688	2.8398					
C_p (J K^{-1}mol^{-1})	199.2	210.49					

TABLE 42.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	35	35	0.733	3.02–2	0.15	7.68–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
180.1–309.7	536.05	9.75637+1	3.43192	8.84349	1.35181+2	−1.40672+2	3.17998+2	III

Name: 2–Methyl–1–propanol
Formula: $C_4H_{10}O$

CAS–RN: 78–83–1
Group No.: 42–017
Molar Mass: 74.12

TABLE 42.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*86SCH		308.6–328.1	9S	nosp	not specified	C_{avg}	DSIO	*86SCH
*98LOU	N	337.9	1	nosp	not specified	C_{avg}	DSIO	*98LOU
24WIL/DAN		303.0–353.0	eqn	nosp	not specified	C_p	BSAO	24WIL/DAN
41ZHD		278.3–319.0	3	nosp	not specified	C_p	BSIT	34KOL/UDO2
58SWI/ZIE2	N	333.6–336.7	2	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
60SWI/ZIE	N	322.6	1	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
68COU/LEE		180.0–355.0	65	0.15	99.96 melpt	C_p	BSAO	63AND/COU1
68PAZ/REC	N	301.1–313.1	2	nosp	not specified	C_p	BDCT	70PAZ/PAZ
77HOF/SAN	N	383.1–493.1	12S	1.00	not specified	C_p	FSIO	75SAN
78RYB/EME		293.1–353.1	7S	nosp	not specified	C_p	BSIO	78RYB/EME
86KOR/KUK		298.0	1	0.20	not specified	C_p	BSAO	83KUK/KOR
88OKA/OGA	N	298.1	1	nosp	not specified	C_p	FSIO	85OGA
88PIE/SOM1		298.1	1	nosp	99.5 chrom	C_p	FSIT	71PIC/LED

*98LOU average value in temperature range 294–382 K
58SWI/ZIE2 average values in temperature ranges 295–372 K and 295–379 K
60SWI/ZIE average value in temperature range 294–351 K
68PAZ/REC same data in 70PAZ/PAZ
77HOF/SAN C_p at saturation curve extrapolated from high pressure measurements
88OKA/OGA water content below 0.083 mol.%

TABLE 42.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68COU/LEE	180.0–355.0	65	0.15	0.852	2.79–2	0.13	–4.02–5	–13
77HOF/SAN	383.1–493.1	12	1.00	0.308	1.02–1	0.31	2.10–2	4
88OKA/OGA	298.1	1	0.40#	0.129	1.13–2	0.05	1.13–2	1
				Rejected data				
*86SCH	(1.91–1, 0.77, 1.69–1, 9)			*98LOU	(4.72–1, 1.77, 4.72–1, 1)			
24WIL/DAN	(6.31–1, 2.26, 5.19–1, 4)			41ZHD	(4.38–1, 1.87, 3.28–1, 1)			
58SWI/ZIE2	(1.40–1, 0.54, 1.38–1, 2)			60SWI/ZIE	(2.62–1, 1.08, –2.62–1, –1)			
68PAZ/REC	(8.34–1, 3.41, 6.93–1, 2)			78RYB/EME	(5.33–1, 2.04, –3.71–1, –3)			
86KOR/KUK	(5.67–2, 0.26, 5.67–2, 1)			88PIE/SOM1	(1.27–1, 0.58, 1.27–1, 1)			

TABLE 42.17.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	109	78	0.820	4.95–2	0.17	3.35–3	–8
C_{sat}	109	78	0.820	4.47–2	0.16	3.18–3	–7

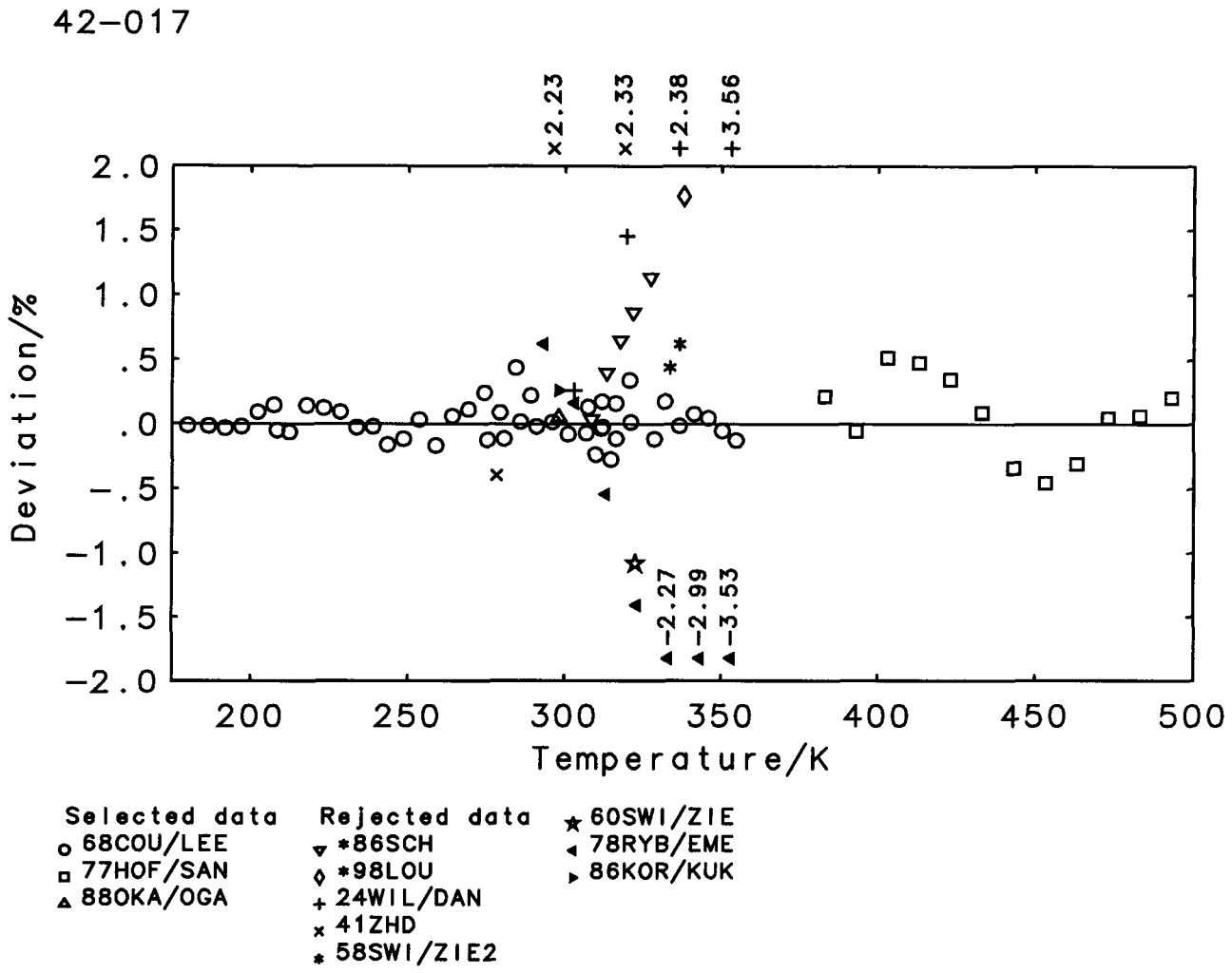
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
180.0–290.0	7.05908	1.17793+1	–6.41903	1.38281	II
290.0–370.0	1.59857+2	–1.46288+2	4.80868+1	–4.88223	II
370.0–493.1	–2.10971+2	1.54384+2	–3.31759+1	2.43873	V
180.0–290.0	7.09018	1.17405+1	–6.40324	1.38070	II
290.0–370.0	1.60179+2	–1.46627+2	4.82062+1	–4.89624	II
370.0–493.1	–1.89033+2	1.36518+2	–2.83193+1	1.99795	V

TABLE 42.17.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p ($J K^{-1} g^{-1}$)	1.742	1.767	1.795	1.828	1.865	1.909	1.960
C_p ($J K^{-1} mol^{-1}$)	129.1	131.0	133.1	135.5	138.3	141.5	145.3
c_{sat} ($J K^{-1} g^{-1}$)	1.742	1.767	1.795	1.828	1.865	1.909	1.960
C_{sat} ($J K^{-1} mol^{-1}$)	129.1	131.0	133.1	135.5	138.3	141.5	145.3
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	2.018	2.086	2.163	2.190	2.251	2.351	2.441
C_p ($J K^{-1} mol^{-1}$)	149.6	154.6	160.4	162.3	166.9	174.3	181.0
c_{sat} ($J K^{-1} g^{-1}$)	2.019	2.086	2.163	2.190	2.251	2.351	2.441
C_{sat} ($J K^{-1} mol^{-1}$)	149.6	154.6	160.4	162.3	166.9	174.3	181.0
Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1} g^{-1}$)	2.463	2.584	2.711	2.840	2.969	3.095	3.213
C_p ($J K^{-1} mol^{-1}$)	182.5	191.5	200.9	210.5	220.1	229.4	238.1
c_{sat} ($J K^{-1} g^{-1}$)	2.463	2.584	2.711	2.840	2.969	3.094	3.212
C_{sat} ($J K^{-1} mol^{-1}$)	182.5	191.5	200.9	210.5	220.1	229.3	238.1
Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1} g^{-1}$)	3.320	3.42	3.50	3.57	3.63	3.69	3.74
C_p ($J K^{-1} mol^{-1}$)	246.1	253	259	265	269	274	277
c_{sat} ($J K^{-1} g^{-1}$)	3.319	3.41	3.50	3.57	3.63	3.68	3.73
C_{sat} ($J K^{-1} mol^{-1}$)	246.0	253	259	264	269	273	276
Temp. (K)	440	450	460	470	480	490	
c_p ($J K^{-1} g^{-1}$)	3.79	3.83	3.88	3.92	3.97	4.02	
C_p ($J K^{-1} mol^{-1}$)	281	284	287	291	294	298	
c_{sat} ($J K^{-1} g^{-1}$)	3.77	3.80	3.83	3.87	3.90	3.93	
C_{sat} ($J K^{-1} mol^{-1}$)	279	282	284	287	289	291	

TABLE 42.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	109	78	21.640	1.10	4.07	9.30–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
180.0–493.1	547.78	–4.62107	1.98647–1	3.32197	2.68746+1		VI



Name: 2–Methyl–2–propanol
Formula: $C_4H_{10}O$

CAS–RN: 75–65–0
Group No.: 42–018
Molar Mass: 74.12

TABLE 42.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26PAR/AND		300.0–300.3	2	nosp	not specified		C_p	BSIO	25PAR
59KEN/TOM		304.6–324.6	2	nosp	not specified		C_p	BSIO	57KEN
61ROU		304.3–316.7	6	nosp	not specified		C_p	BSAO	61ROU
63OET		303.6–331.3	12	0.30	99.91	melpt	C_p	BSAO	58HIL/KRA
71REC/SAD		303.1	1	nosp	not specified		C_p	BSIO	70REC
76SKO/SUU		298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
77DEV/PER1		298.1–328.1	3	nosp	not specified		C_p	FSIT	71PIC/LED
77DEV/PER2		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
77HOF/SAN	N	353.1–453.1	11S	1.00	not specified		C_p	FSIO	75SAN
77MUR/SUB		298.1	1	0.30	not specified		C_p	BSIO	64MOE/THO
88OKA/OGA	N	298.1	1	nosp	not specified		C_p	FSIO	85OGA

77HOF/SAN C_p at saturation curve extrapolated from high pressure measurements
88OKA/OGA water content below 0.083 mol.%

TABLE 42.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
63OET	303.6–331.3	12	0.30	0.371	3.12–2	0.11	2.14–3	2
76SKO/SUU	298.1	1	0.10	0.181	4.75–3	0.02	–4.75–3	–1
77HOF/SAN	353.1–453.1	11	1.00	0.280	8.97–2	0.28	1.87–2	1
				Rejected data				
26PAR/AND	(5.32–1, 1.96, 5.31–1, 2)			59KEN/TOM	(1.11, 4.17,–1.11, –2)			
61ROU	(2.23–1, 0.80, 1.81–1, 4)			71REC/SAD	(2.05–1, 0.75, 2.05–1, 1)			
77DEV/PER1	(6.16–1, 2.42,–3.47–1, –1)			77DEV/PER2	(1.04, 4.11,–1.04, –1)			
77MUR/SUB	(7.53–1, 2.78, 7.53–1, 1)			88OKA/OGA	(3.90–1, 1.46, 3.90–1, 1)			

TABLE 42.18.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	24	0.366	7.26–2	0.23	9.42–3	2
C_{sat}	41	24	0.365	7.43–2	0.23	7.75–3	4

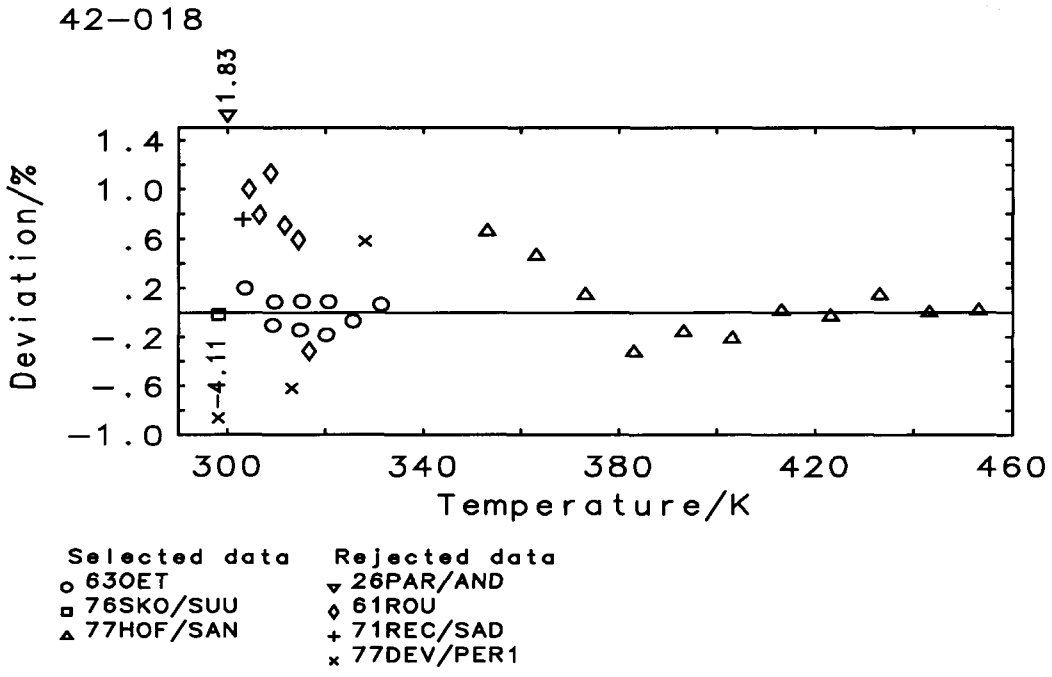
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–330.0	–4.49679+2	4.06731+2	–1.16848+2	1.13952+1	II
330.0–453.1	–1.00397+2	8.92015+1	–2.06274+1	1.67587	V
298.1–330.0	–4.82832+2	4.37822+2	–1.26544+2	1.24004+1	II
330.0–453.1	–7.39444+1	6.61058+1	–1.39028+1	1.02251	V

TABLE 42.18.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.978	3.112	3.223	3.316	3.40	3.47	3.54
C_p (J K^{-1}mol^{-1})	220.7	230.7	238.9	245.8	252	258	263
c_{sat} (J K^{-1}g^{-1})	2.978	3.113	3.222	3.315	3.40	3.47	3.54
C_{sat} (J K^{-1}mol^{-1})	220.7	230.7	238.8	245.7	252	257	262
Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	3.61	3.66	3.72	3.77	3.82	3.87	3.93
C_p (J K^{-1}mol^{-1})	267	272	276	280	283	287	291
c_{sat} (J K^{-1}g^{-1})	3.60	3.66	3.71	3.75	3.80	3.84	3.87
C_{sat} (J K^{-1}mol^{-1})	267	271	275	278	281	284	287
Temp. (K)	440	450					
c_p (J K^{-1}g^{-1})	3.98	4.04					
C_p (J K^{-1}mol^{-1})	295	299					
c_{sat} (J K^{-1}g^{-1})	3.91	3.95					
C_{sat} (J K^{-1}mol^{-1})	290	292					

TABLE 42.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	24	0.900	8.50–2	0.26	8.61–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
298.1–453.1	506.21	1.34853+1	1.12394	–1.20033+2	5.33422+2	–6.12221+2	2.63702+2	V



Name: 1,3–Butanediol
Formula: $C_4H_{10}O_2$

CAS–RN: 107–88–0
Group No.: 42–019
Molar Mass: 90.12

TABLE 42.19.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72KAW/OTA	303.15	2.524	nosp	not specified		C_p	BSIO	49WEI

Name: 1,4–Butanediol
Formula: $C_4H_{10}O_2$

CAS–RN: 110–63–4
Group No.: 42–020
Molar Mass: 90.12

TABLE 42.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74PET/TER	297.8–431.9	14	1.00	98.	melpt	C_p	BDCT	74PET/TER
79NIS/BAB	295.7–315.8	16	0.30	99.48	melpt	C_p	BSAO	76LEB/LIT
79NIS/BAB	310.0–450.0	15	0.80	99.48	melpt	C_p	BSAO	68LEA

TABLE 42.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79NIS/BAB	295.7–315.8	16	0.30	0.239	1.77–2	0.07	1.45–3	0
79NIS/BAB	310.0–450.0	15	0.80	0.214	4.98–2	0.17	−1.06–2	−1
				Rejected data				
74PET/TER	(1.61, 6.56,–1.53, −14)							

TABLE 42.20.3. Parameters of regression polynomial

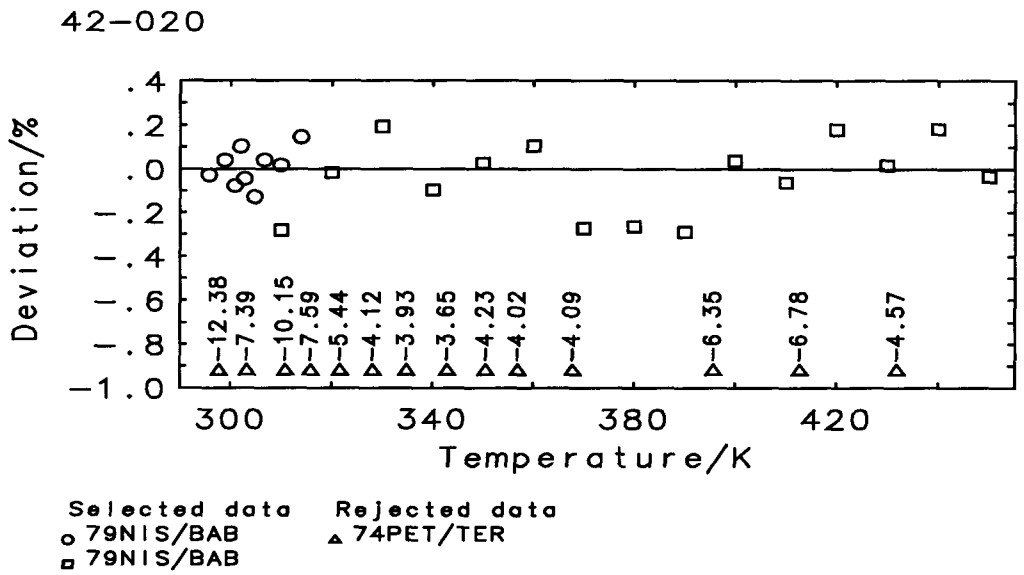
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	31	0.239	3.88–2	0.14	−4.39–3	−1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
295.7–450.0		9.84360	3.17147	5.38102–1			IV

TABLE 42.20.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1} g^{-1}$)	2.233	2.292	2.353	2.414	2.477	2.540	2.605
C_p ($J K^{-1} mol^{-1}$)	201.2	206.6	212.0	217.6	223.2	228.9	234.8
Temp. (K)	370	380	390	400	410	420	430
c_p ($J K^{-1} g^{-1}$)	2.670	2.737	2.804	2.873	2.942	3.013	3.084
C_p ($J K^{-1} mol^{-1}$)	240.7	246.7	252.7	258.9	265.2	271.5	278.0
Temp. (K)	440	450					
c_p ($J K^{-1} g^{-1}$)	3.157	3.230					
C_p ($J K^{-1} mol^{-1}$)	284.5	291.1					

TABLE 42.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	45	31	0.236	3.71–2	0.13	1.99–3	7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
295.7–450.0	707.00	–9.67799	9.01507–1	6.26388	2.59742+1		IV



Name: 2,3–Butanediol
Formula: $C_4H_{10}O_2$

CAS–RN: 513–85–9
Group No.: 42–021
Molar Mass: 90.12

TABLE 42.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36KHO/KAL	N	316.2–357.6	7	nosp	not specified		C_{avg}	DSIO	36KHO/KAL

36KHO/KAL maximum water content 0.1 %

TABLE 42.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	7	7	0.002	1.77–3	0.01	1.63–6	0

Temp. range K	A_1	A_2	Level of uncertainty
316.2–357.6	–2.19303	9.31591	VI

TABLE 42.21.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360
c ($J\,K^{-1}g^{-1}$)	2.55	2.63	2.72	2.81	2.89
C ($J\,K^{-1}mol^{-1}$)	230	237	245	253	261

Name: (*R**,*S**)–1,2,3,4–Butanetetrol
Formula: $C_4H_{10}O_4$

CAS–RN: 149–32–6
Group No.: 42–022
Molar Mass: 122.12

TABLE 42.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
32SPA/THO	403.1–423.1	3S	nosp	not specified		C_p	BDHO	31THO/PAR

TABLE 42.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
403.1–423.1	2.95853+1	3.07264	V

TABLE 42.22.4. Recommended values of heat capacities

Temp. (K)	400	410	420
c_p ($J\,K^{-1}g^{-1}$)	2.85	2.87	2.89
C_p ($J\,K^{-1}mol^{-1}$)	348	351	353

Name: Cyclopentanol
Formula: $C_5H_{10}O$

CAS-RN: 96-41-3
Group No.: 42-023
Molar Mass: 86.13

TABLE 42.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56PAR/KEN	260.0–300.0	5S	1.00	99.8	melpt	C_p	BSIO	25PAR
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
86BEN/DAR2	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 42.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56PAR/KEN	260.0–300.0	5	1.00	0.418	8.37–2	0.42	–4.07–2	–3
76CON/GIA	298.1	1	0.70#	0.661	1.03–1	0.46	1.03–1	1
				Rejected data				
86BEN/DAR2	(3.52–1, 1.61,–3.52–1, –1)							

TABLE 42.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.572	1.07–1	0.52	–1.67–2	–2
Temp. range K		A_1	A_2				Level of uncertainty
260.0–300.0		–6.00319	9.45580				IV

TABLE 42.23.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	1.794	1.885	1.914	1.976	2.068	2.142	2.159
C_p ($J\,K^{-1}mol^{-1}$)	154.5	162.4	164.8	170.2	178.1	184.5	185.9

Name: 2-Methyl-3-buten-2-ol
Formula: $C_5H_{10}O$

CAS-RN: 115-18-4
Group No.: 42-024
Molar Mass: 86.13

TABLE 42.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84BAG/BAE	N	273.3–343.4	5	0.80	99.	estim	C_p	BDHT	86CDA/COM

84BAG/BAE same data in 86BER/GUR and 88BAG/GUR

TABLE 42.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.557	1.30–1	0.45	3.55–4	1
Temp. range K		A_1	A_2				Level of uncertainty
273.3–343.4		5.21875	7.90741				V

TABLE 42.24.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	2.56	2.59	2.64	2.72	2.78	2.79	2.87
C_p ($J K^{-1}mol^{-1}$)	221	223	227	234	239	241	247
Temp. (K)	320	330	340				
c_p ($J K^{-1}g^{-1}$)	2.95	3.02	3.10				
C_p ($J K^{-1}mol^{-1}$)	254	260	267				

Name: 2–Methyl–1–butanol
Formula: $C_5H_{12}O$

CAS–RN: 137–32–6
Group No.: 42–025
Molar Mass: 88.15

TABLE 42.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*98LOU	N	347.1	1	nosp	not specified		C_{avg}	DSIO	*98LOU
49LEE		313.0–343.0	eqn	nosp	not specified		C_p	BDHO	33FER/MIL
94SVO/CEJ		303.0–326.2	6	0.50	99.8	chrom	C_p	BSAO	91SVO/ZAB1

*98LOU average value in temperature range 295–400 K

TABLE 42.25.2. Correlated heat capacities

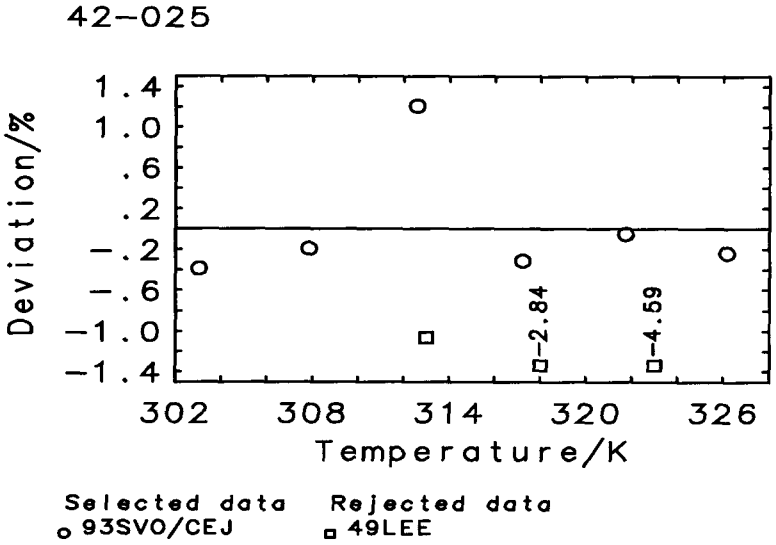
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
93SVO/CEJ	303.0–326.2	6	0.50	1.098	1.52–1	0.55	1.53–3	–4
				Rejected data				
49LEE	(8.83–1, 3.18,–7.85–1, –3)							

TABLE 42.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	6	1.344	1.86–1	0.67	1.53–3	–4
Temp. range K		A_1	A_2				Level of uncertainty
303.0–326.2		–2.06485+1	1.54090+1				IV

TABLE 42.25.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	2.413	2.558	2.703	2.849
C_p ($J K^{-1} mol^{-1}$)	212.7	225.5	238.3	251.1



Name: 2–Methyl–2–butanol
Formula: $C_5H_{12}O$

CAS–RN: 75–85–4
Group No.: 42–026
Molar Mass: 88.15

TABLE 42.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*98LOU	N	332.4	1	nosp	not specified		C_{avg}	DSIO	*98LOU
33PAR/HUF		275.0–294.4	4	1.00	not specified		C_p	BSIO	25PAR
49LEE		313.0–343.0	eqn	nosp	not specified		C_p	BDHO	33FER/MIL
83DAP/DEL		288.1–298.1	2	0.30	not specified		C_p	FSIT	71PIC/LED
86BEN/DAR2		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
88PIE/SOM1		298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED
94SVO/CEJ		303.0–326.2	6	0.50	98.8	chrom	C_p	BSAO	91SVO/ZAB1

*98LOU average value in temperature range 293–372 K

TABLE 42.26.2. Correlated heat capacities

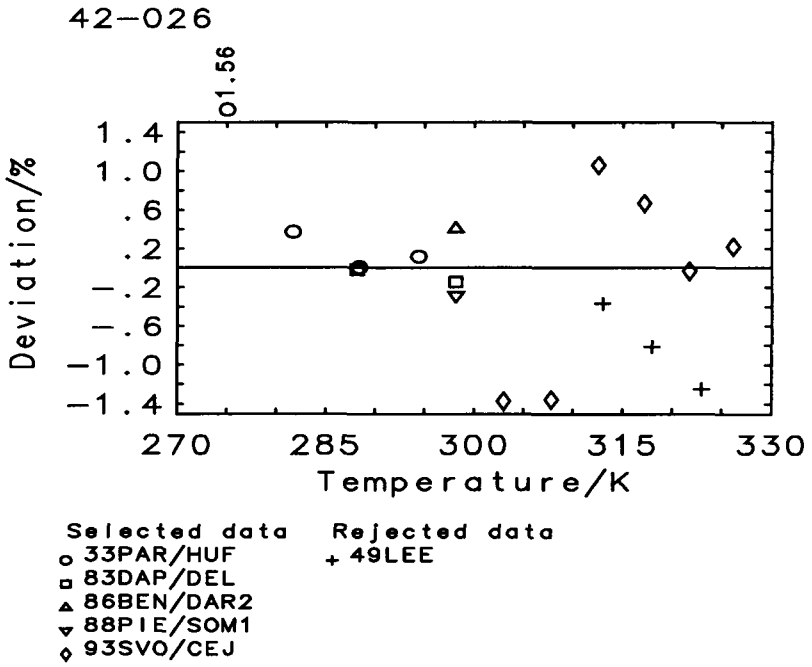
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33PAR/HUF	275.0–294.4	4	1.00	0.804	2.20–1	0.80	1.41–1	3
83DAP/DEL	288.1–298.1	2	0.30	0.344	3.07–2	0.10	–2.41–2	–2
86BEN/DAR2	298.1	1	0.30	1.342	1.20–1	0.40	1.20–1	1
88PIE/SOM1	298.1	1	0.50#	0.573	8.52–2	0.29	–8.52–2	–1
93SVO/CEJ	303.0–326.2	6	0.50	1.886	2.91–1	0.94	–3.54–2	0
				Rejected data				
49LEE	(2.88–1, 0.89,–2.62–1, –3)							

TABLE 42.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	14	1.480	2.46–1	0.83	2.41–2	1
Temp. range K		A_1	A_2				Level of uncertainty
275.0–326.2		–8.25642	1.27676+1				IV

TABLE 42.26.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.473	2.511	2.593	2.714	2.812	2.834	2.954
C_p (J K^{-1}mol^{-1})	218.0	221.3	228.6	239.2	247.9	249.8	260.4
Temp. (K)	320	330					
c_p (J K^{-1}g^{-1})	3.075	3.195					
C_p (J K^{-1}mol^{-1})	271.1	281.7					



Name: 3–Methyl–1–butanol
Formula: $C_5H_{12}O$

CAS–RN: 123–51–3
Group No.: 42–027
Molar Mass: 88.15

TABLE 42.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH		309.7–337.4	10S	nosp	not specified		C_{avg}	DSIO	*86SCH
*98LOU	N	348.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
07BAT		224.0–263.6	6	nosp	not specified		C_p	BSIO	07BAT
12LUS	N	321.0	1	nosp	not specified		C_{avg}	DSIO	12LUS
24WIL/DAN		303.0–353.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
45ZHD		280.5–319.9	3	nosp	not specified		C_p	BSIT	34KOL/UDO2
49LEE		313.0–343.0	eqn	nosp	not specified		C_p	BDHO	33FER/MIL
58SWI/ZIE2	N	347.5	1	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1
90RAO/RAJ		318.1–333.1	4	4.00	not specified		C_p	BDHT	89PRA/RAJ
94SVO/CEJ		303.0–326.2	6	0.50	100.0	chrom	C_p	BSAO	91SVO/ZAB1

*98LOU average value in temperature range 294–403 K
12LUS average value in temperature range 287–355 K
58SWI/ZIE2 average value in temperature range 295–400 K

TABLE 42.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
07BAT	224.0–263.6	6	3.00#	0.241	1.54–1	0.72	–2.68–2	0
58SWI/ZIE2	347.5	1	1.00#	0.141	4.38–2	0.14	–4.38–2	–1
93SVO/CEJ	303.0–326.2	6	0.50	1.039	1.40–1	0.52	3.97–3	–2
				Rejected data				
*86SCH	(3.94–1, 1.39, 3.90–1, 10)			12LUS	(1.85, 6.30, 1.85, 1)			
24WIL/DAN	(4.28–1, 1.54,–4.18–1, –5)			45ZHD	(2.99–1, 1.18, 2.80–1, 3)			
49LEE	(4.54–1, 1.56,–1.74–1, 0)			90RAO/RAJ	(1.14, 4.33,–1.01, –4)			

TABLE 42.27.3. Parameters of regression polynomial

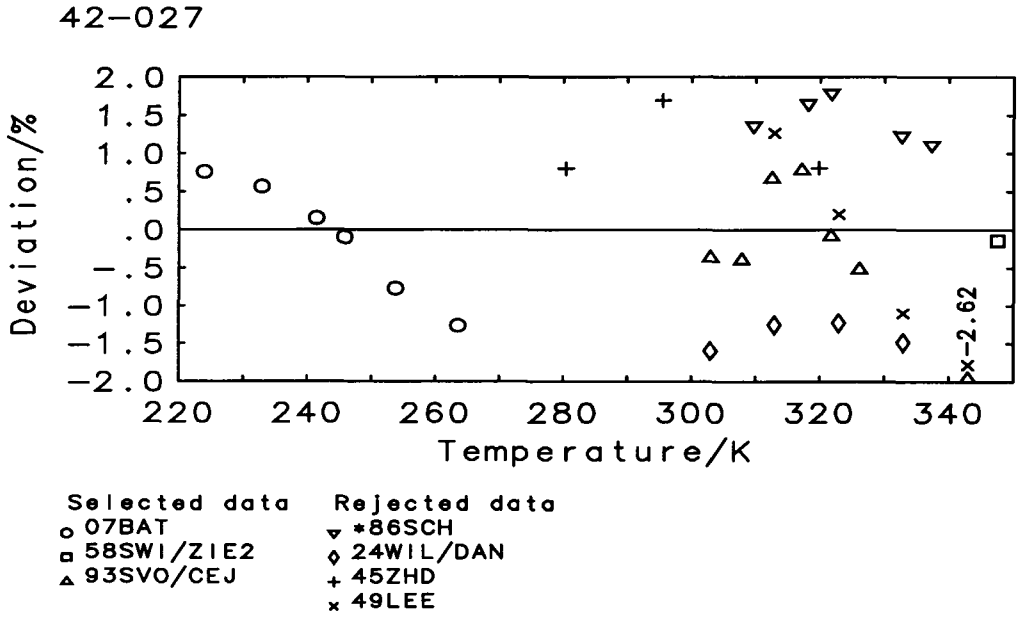
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	42	13	0.827	1.62–1	0.69	–1.39–2	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
224.0–347.5		3.42886+1	–1.62165+1	4.39785			IV

TABLE 42.27.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.877	1.911	1.953	2.003	2.061	2.128	2.151
C_p (J K^{-1}mol^{-1})	165.4	168.4	172.1	176.5	181.7	187.6	189.6
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.204	2.287	2.361	2.379	2.479	2.587	2.704
C_p (J K^{-1}mol^{-1})	194.2	201.6	208.1	209.7	218.5	228.1	238.4
Temp. (K)	340	350					
c_p (J K^{-1}g^{-1})	2.829	2.962					
C_p (J K^{-1}mol^{-1})	249.4	261.1					

TABLE 42.27.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	42	13	0.852	1.51–1	0.63	–2.27–2	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
224.0–347.5	579.40	7.78925+2	6.15988+1	–5.31475+1	8.44602+2	–1.82150+2	9.38305+2	IV



Name: 3–Methyl–2–butanol
Formula: $C_5H_{12}O$

CAS–RN: 598–75–4
Group No.: 42–028
Molar Mass: 88.15

TABLE 42.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
94SVO/CEJ	303.0–326.2	6	0.50	99.6	chrom	C_p	BSAO	91SVO/ZAB1

TABLE 42.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.369	2.14–1	0.68	1.84–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
303.0–326.2		–8.56897	1.25857+1				IV

TABLE 42.28.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	2.753	2.872	2.991	3.109
C_p ($J K^{-1} mol^{-1}$)	242.7	253.2	263.6	274.1

Name: 1–Pentanol
Formula: $C_5H_{12}O$

CAS–RN: 71–41–0
Group No.: 42–029
Molar Mass: 88.15

TABLE 42.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
33PAR/HUF		204.1–298.0	6	1.00	not specified	C_p	BSIO	25PAR
39PHI	N	302.4	1	nosp	not specified	C_p	BSIO	49WEI
49LEE		313.0–343.0	eqn	nosp	not specified	C_p	BDHO	33FER/MIL
49TSC/RIC2		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
68COU/LEE		205.1–389.1	53	0.15	99.87 melpt	C_p	BSAO	63AND/COU1
68PAZ/REC	N	313.1	1	nosp	not specified	C_p	BDCT	70PAZ/PAZ
76SKO/SUU		298.1	1	0.10	not specified	C_p	DDCT	71KON/SUU
79GRI/YAN	N	301.3–463.4	9	0.90	not specified	C_p	BDAO	75RAS/GRI
81ARU/BAG		293.1–393.1	6S	1.50	not specified	C_p	BDHT	81ARU
83DAP/DEL		288.1–298.1	2	0.30	not specified	C_p	FSIT	71PIC/LED
86BEN/DAR2		298.1	1	0.30	not specified	C_p	FSIT	71PIC/LED
86TAN/TOY		298.1	1	0.30	98. anal	C_p	FSIT	71PIC/LED

39PHI isomer not specified, 1–alkanol assumed
68PAZ/REC same datum in 70PAZ/PAZ
79GRI/YAN data above 382.68 K were measured at elevated pressures up to 0.81 MPa

TABLE 42.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68COU/LEE	205.1–389.1	53	0.15	0.386	1.41–2	0.06	–1.97–3	–4
76SKO/SUU	298.1	1	0.10	1.229	3.08–2	0.12	3.08–2	1
79GRI/YAN	301.3–463.4	9	0.90	0.697	2.00–1	0.63	1.41–1	5
86TAN/TOY	298.1	1	0.30	0.074	5.56–3	0.02	5.56–3	1
				Rejected data				
33PAR/HUF	(7.74–2, 0.31, 6.67–2, 5)			39PHI	(1.18, 4.87,–1.18, –1)			
49LEE	(1.54, 5.67,–1.46, –5)			49TSC/RIC2	(6.94–1, 2.70, 6.94–1, 1)			
68PAZ/REC	(2.35, 8.12, 2.35, 1)			81ARU/BAG	(3.93–1, 1.36,–2.93–1, –4)			
83DAP/DEL	(7.88–2, 0.32,–7.37–2, –2)			86BEN/DAR2	(8.34–2, 0.33, –8.34–2, –1)			

TABLE 42.29.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	87	64	0.488	8.01–2	0.25	1.88–2	3
C_{sat}	87	64	0.487	8.02–2	0.25	1.89–2	4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
205.1–295.0	1.17766+1	1.05999+1	–5.86906	1.27627	II
295.0–380.0	1.62500+2	–1.42678+2	4.60895+1	–4.59475	II
380.0–463.4	–2.84074+2	2.09881+2	–4.66891+1	3.54372	IV
205.1–295.0	1.16046+1	1.08050+1	–5.94967	1.28672	II
295.0–380.0	1.63346+2	–1.43508+2	4.63599+1	–4.62397	II
380.0–463.4	–2.79379+2	2.06012+2	–4.56190+1	3.44437	IV

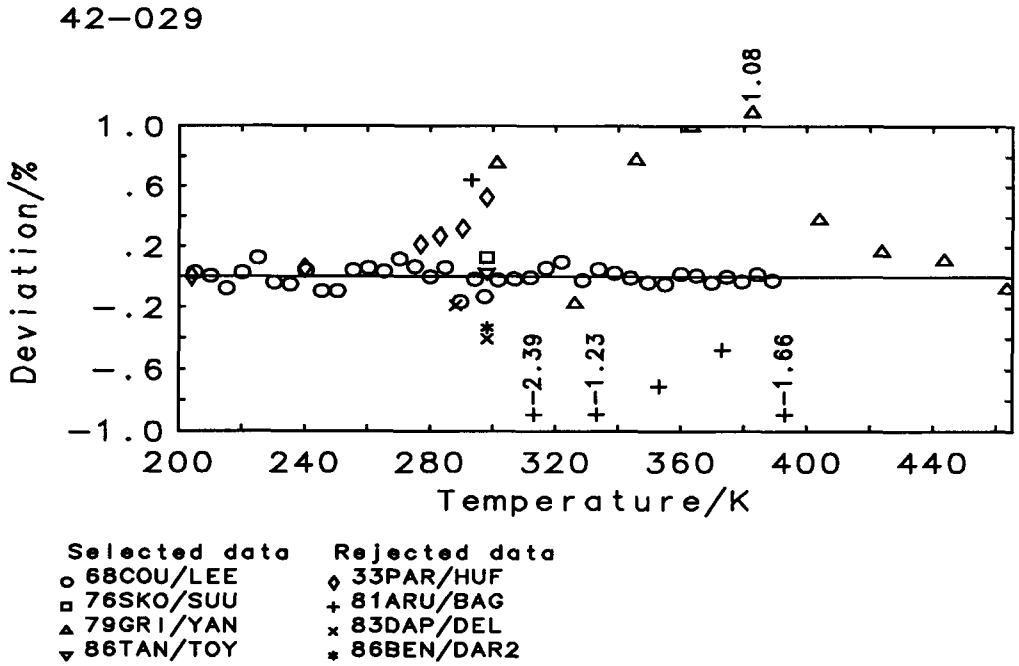
TABLE 42.29.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J\,K^{-1}g^{-1}$)	1.884	1.913	1.947	1.986	2.031	2.084	2.144
C_p ($J\,K^{-1}mol^{-1}$)	166.1	168.6	171.6	175.1	179.1	183.7	189.0
c_{sat} ($J\,K^{-1}g^{-1}$)	1.884	1.913	1.947	1.986	2.031	2.084	2.144
C_{sat} ($J\,K^{-1}mol^{-1}$)	166.1	168.6	171.6	175.1	179.1	183.7	189.0
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	2.165	2.213	2.291	2.361	2.378	2.475	2.577
C_p ($J\,K^{-1}mol^{-1}$)	190.8	195.1	201.9	208.1	209.6	218.1	227.2
c_{sat} ($J\,K^{-1}g^{-1}$)	2.165	2.213	2.291	2.361	2.378	2.475	2.578
C_{sat} ($J\,K^{-1}mol^{-1}$)	190.8	195.1	201.9	208.1	209.6	218.1	227.2
Temp. (K)	330	340	350	360	370	380	390
c_p ($J\,K^{-1}g^{-1}$)	2.684	2.792	2.898	3.000	3.096	3.182	3.257
C_p ($J\,K^{-1}mol^{-1}$)	236.6	246.1	255.5	264.5	272.9	280.5	287.1
c_{sat} ($J\,K^{-1}g^{-1}$)	2.684	2.792	2.898	3.000	3.095	3.181	3.256
C_{sat} ($J\,K^{-1}mol^{-1}$)	236.6	246.1	255.5	264.4	272.8	280.4	287.0
Temp. (K)	400	410	420	430	440	450	460
c_p ($J\,K^{-1}g^{-1}$)	3.322	3.380	3.431	3.479	3.525	3.571	3.619
C_p ($J\,K^{-1}mol^{-1}$)	292.8	297.9	302.5	306.7	310.7	314.8	319.0
c_{sat} ($J\,K^{-1}g^{-1}$)	3.320	3.377	3.427	3.474	3.518	3.561	3.607
C_{sat} ($J\,K^{-1}mol^{-1}$)	292.7	297.7	302.1	306.2	310.1	313.9	317.9

TABLE 42.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	87	64	2.604	2.34–1	0.67	–6.06–2	–4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
205.1–463.4	588.15	8.68173+2	7.33854+1	–6.24976+1	9.01687+2	–9.29696+1	9.16830+2	IV



Name: 2–Pentanol
Formula: $C_5H_{12}O$

CAS–RN: 6032–29–7
Group No.: 42–030
Molar Mass: 88.15

TABLE 42.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		C_p	not specified	
94SVO/CEJ		303.0–326.2	6	0.50	99.6	chrom	C_p	BSAO	91SVO/ZAB1

38PAN/DUD temperature range of parameters validity estimated by the compilers

TABLE 42.30.2. Correlated heat capacities

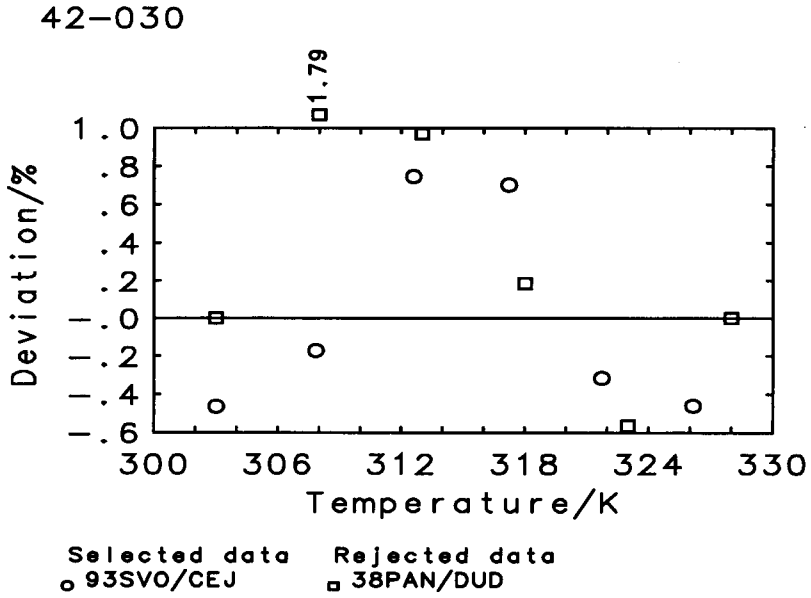
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
93SVO/CEJ	303.0–326.2	6	0.50	1.036	1.58–1	0.52	1.45–3	–2
				Rejected data				
38PAN/DUD	(3.19–1, 1.06, 1.76–1, 2)							

TABLE 42.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	6	1.268	1.93–1	0.63	1.45–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
303.0–326.2		–1.76616+1	1.52434+1				IV

TABLE 42.30.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p (J K^{-1}g^{-1})	2.648	2.791	2.935	3.079
C_p (J K^{-1}mol^{-1})	233.4	246.1	258.7	271.4



Name: 3-Pentanol
Formula: $C_5H_{12}O$

CAS-RN: 584-02-1
Group No.: 42-031
Molar Mass: 88.15

TABLE 42.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49LEE	313.0–343.0	eqn	nosp	not specified		C_p	BDHO	33FER/MIL
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
94SVO/CEJ	303.0–326.2	6	0.50	99.6	chrom	C_p	BSAO	91SVO/ZAB1

TABLE 42.31.2. Correlated heat capacities

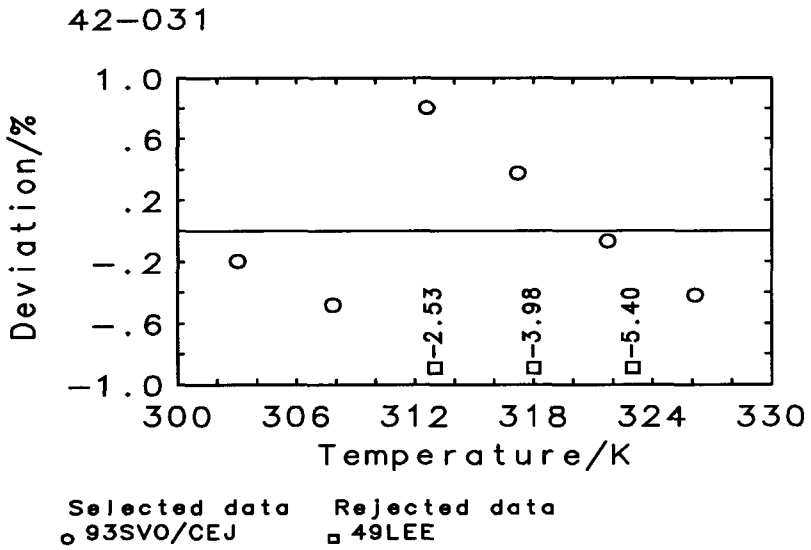
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
93SVO/CEJ	303.0–326.2	6	0.50	0.908	1.45–1	0.45	1.21–3	–2
				Rejected data				
49LEE	(1.29, 4.14,–1.24, –3)							

TABLE 42.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	6	1.112	1.77–1	0.56	1.21–3	–2
Temp. range K		A_1	A_2				Level of *uncertainty*
303.0–326.2		–1.07635+1	1.35500+1				IV

TABLE 42.31.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p (J K^{-1}g^{-1})	2.819	2.947	3.075	3.202
C_p (J K^{-1}mol^{-1})	248.5	259.8	271.0	282.3



Name: 2,2–Dimethyl–1,3–propanediol
Formula: $C_5H_{12}O_2$

CAS–RN: 126–30–7
Group No.: 42–032
Molar Mass: 104.15

TABLE 42.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
88ZHA/ZOU	410.0–440.0	4S	nosp	not specified	C_p	BSAO	88ZHA/ZOU

TABLE 42.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.000	1.43–5	0.00	5.72–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
410.0–440.0		–1.07511+2	6.51092+1	–7.15618			IV

TABLE 42.32.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440
c_p (J K^{-1}g^{-1})	3.125	3.170	3.205	3.227
C_p (J K^{-1}mol^{-1})	325.4	330.2	333.8	336.1

Name: 1,5–Pentanediol
Formula: $C_5H_{12}O_2$

CAS–RN: 111–29–5
Group No.: 42–033
Molar Mass: 104.15

TABLE 42.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
34MIL	N	269.8–287.0	2	nosp	not specified	C_{avg}	BSIO	20GIB/LAT

34MIL average values in temperature ranges 253–287 K and 271–303 K

TABLE 42.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
269.8–287.0		4.45988–1	8.60994				V

TABLE 42.33.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15
c (J K^{-1}g^{-1})	1.89	1.91	1.96	2.03	2.08
C (J K^{-1}mol^{-1})	197	199	204	211	217

Name: Phenol
Formula: C_6H_6O

CAS-RN: 108-95-2
Group No.: 42-034
Molar Mass: 94.11

TABLE 42.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
27FER	345.1–345.1	2	nosp	not specified	C_p	BSIO	27FER
59LUT/PAN	336.0–402.0	eqn	nosp	not specified	C_p	BDHO	58LUT/PAN
63AND/COU1	317.3–335.8	14	0.30	99.96 melpt	C_p	BSAO	63AND/COU1
67RAS/GAN	313.1–373.1	4S	0.50	not specified	C_p	BSAO	67RAS/GAN

TABLE 42.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
63AND/COU1	317.3–335.8	14	0.30	0.712	5.27–2	0.21	9.68–3	0
67RAS/GAN	313.1–373.1	4	0.50	1.230	1.52–1	0.62	–9.00–2	–2
				Rejected data				
27FER	(8.50–1, 3.28, 8.50–1, 2)			59LUT/PAN	(1.59, 5.91, 1.57, 3)			

TABLE 42.34.3. Parameters of regression polynomial

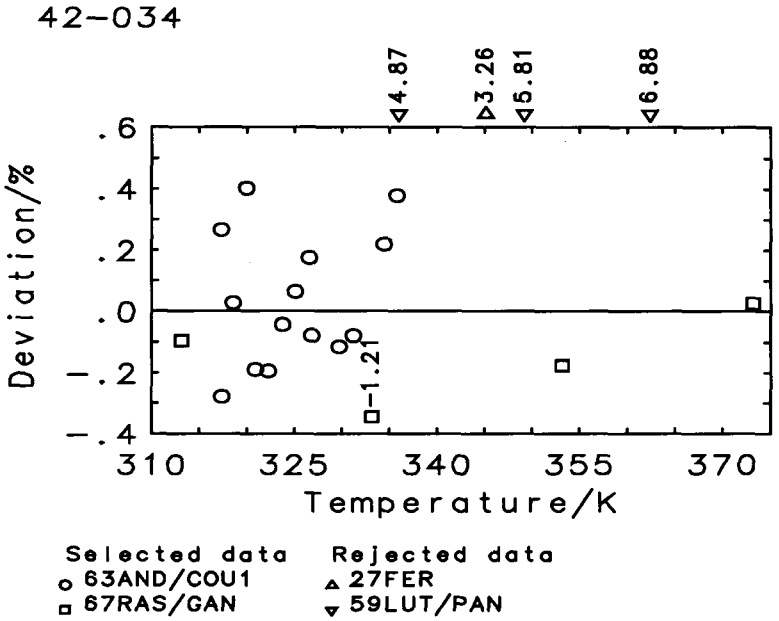
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	18	0.969	9.66–2	0.39	–1.25–2	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
313.1–373.1		–6.67058+2	5.95564+2	–1.71181+2	1.64370+1		III

TABLE 42.34.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.161	2.194	2.213	2.225	2.240	2.266
C_p (J K^{-1}mol^{-1})	203.4	206.5	208.3	209.4	210.8	213.2

TABLE 42.34.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	18	1.146	1.16–1	0.47	3.19–3	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
313.1–373.1	694.25	3.75122+2	7.66284+1	–9.75266+1	4.59086+2		IV



Name: 1,2–Benzenediol
Formula: $C_6H_6O_2$

CAS–RN: 120–80–9
Group No.: 42–035
Molar Mass: 110.11

TABLE 42.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	378.0–473.0	eqn	nosp	not specified	C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 42.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	1.78–6	0.00	5.72–7	0
Temp. range K		A_1	A_2				Level of uncertainty
378.0–473.4		1.73665+1	3.01930				V

TABLE 42.35.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.18	2.20	2.22	2.25	2.27	2.29	2.31
C_p (J K^{-1}mol^{-1})	240	242	245	247	250	252	255
Temp. (K)	450	460	470				
c_p (J K^{-1}g^{-1})	2.34	2.36	2.38				
C_p (J K^{-1}mol^{-1})	257	260	262				

Name: 1,3–Benzenediol
Formula: $C_6H_6O_2$

CAS–RN: 108–46–3
Group No.: 42–036
Molar Mass: 110.11

TABLE 42.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	383.0–473.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 42.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	1.65–6	0.00	3.82–7	0
Temp. range K		A_1	A_2				Level of uncertainty
383.0–473.0		1.54284+1	3.52252				V

TABLE 42.36.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440	450
c_p ($J\,K^{-1}g^{-1}$)	2.20	2.23	2.26	2.28	2.31	2.34	2.36
C_p ($J\,K^{-1}mol^{-1}$)	243	245	248	251	254	257	260
Temp. (K)	460	470					
c_p ($J\,K^{-1}g^{-1}$)	2.39	2.42					
C_p ($J\,K^{-1}mol^{-1}$)	263	266					

Name: 1,4–Benzenediol
Formula: $C_6H_6O_2$

CAS–RN: 123–31–9
Group No.: 42–037
Molar Mass: 110.11

TABLE 42.37.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	446.0–473.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 42.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	1.56–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
446.0–473.2		2.12264+1	2.21415				V

TABLE 42.37.4. Recommended values of heat capacities

Temp. (K)	450	460	470
c_p (J K^{-1}g^{-1})	2.36	2.37	2.39
C_p (J K^{-1}mol^{-1})	259	261	263

Name: Cyclohexanol
Formula: $C_6H_{12}O$

CAS-RN: 108-93-0
Group No.: 42-038
Molar Mass: 100.16

TABLE 42.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
24HER/BLO	289.6	1	nosp	not specified	C_p	DSIO	22HER/SCH
29KEL4	298.1–298.7	2	0.50	not specified	C_p	BSIO	29KEL1
39PHI	305.0	1	nosp	not specified	C_p	BSIO	49WEI
68ADA/SUG	300.1–316.5	9	nosp	99.975 melpt	C_p	BSAO	65SUG/SEK
74PET/TER	298.0–427.7	13	1.00	99. chrom	C_p	BDCT	74PET/TER
76CON/GIA	298.1	1	nosp	not specified	C_p	BDCT	76CON/GIA
88CAC/COS	298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED

TABLE 42.38.2. Correlated heat capacities

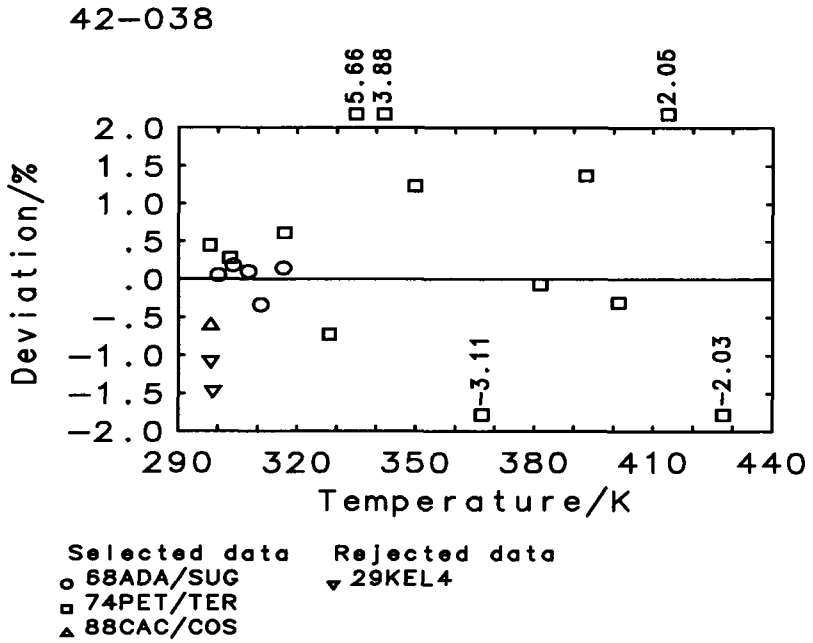
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68ADA/SUG	300.1–316.5	9	0.20#	0.935	5.02–2	0.19	2.13–4	1
74PET/TER	298.0–427.7	13	2.00#	1.158	7.57–1	2.32	2.26–1	3
88CAC/COS	298.1	1	0.50#	1.225	1.55–1	0.61	–1.55–1	–1
				Rejected data				
29KEL4	(3.23–1, 1.28,–3.19–1, –2)			39PHI	(1.94, 7.98,–1.94, –1)			
76CON/GIA	(1.06, 4.00, 1.06, 1)							

TABLE 42.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	23	1.157	6.12–1	1.88	1.21–1	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.0–427.7		–3.14760+1	2.53178+1	–2.09223			V

TABLE 42.38.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.13	2.23	2.33	2.43	2.53	2.62	2.70
C_p (J K^{-1}mol^{-1})	213	224	234	244	253	262	271
Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.79	2.87	2.94	3.01	3.08	3.15	3.21
C_p (J K^{-1}mol^{-1})	279	287	295	302	309	316	322



Name: 3,3–Dimethyl–1–butanol
Formula: $C_6H_{14}O$

CAS–RN: 624–95–3
Group No.: 42–039
Molar Mass: 102.18

TABLE 42.39.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BEN/KUM	298.15	2.311	nosp	99.	chrom	C_p	FSIT	71PIC/LED

Name: 2–Ethyl–1–butanol
Formula: $C_6H_{14}O$

CAS–RN: 97–95–0
Group No.: 42–040
Molar Mass: 102.18

TABLE 42.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85BEN/DAR	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
86ORT	298.1	1	1.00	98.	anal	C_p	BDCT	70PAZ/PAZ

TABLE 42.40.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
85BEN/DAR	298.1	1	0.30	0.000	0.00	0.00	0.00	0
				Rejected data				
86ORT	(7.42–1, 2.50,–7.42–1, –1)							

TABLE 42.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.04071+1	III

TABLE 42.40.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.474
C_p (J K^{-1}mol^{-1})	252.8

Name: 1–Hexanol
Formula: $C_6H_{14}O$

CAS–RN: 111–27–3
Group No.: 42–041
Molar Mass: 102.18

TABLE 42.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
29KEL2		229.6–290.0	7	1.00	not specified		C_p	BSIO	29KEL1
59HUT/BAI		298.1	1	nosp	not specified		C_p	BSIO	55HUT/MAN
73KAL/WOY		303.1	1	nosp	not specified		C_p	BSIO	70REC
79GRI/YAN	N	303.7–462.0	9	0.90	not specified		C_p	BDAO	75RAS/GRI
81ARU		293.1–393.1	6S	1.50	not specified		C_p	BDHT	81ARU
83BEN/DAR		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
84BRA/PIN		298.1	1	nosp	99.	melpt	C_p	FSIT	71PIC/LED
84KAL/WOY		229.1–300.6	35	nosp	99.9	chrom	C_p	BSAO	80KAL/JED
85COS/PAT8		283.1–313.1	3	0.30	98.	estim	C_p	FSIT	71PIC/LED
86ORT		298.1	1	1.00	99.	anal	C_p	BDCT	70PAZ/PAZ
86TAN/TOY		298.1	1	0.30	98.	anal	C_p	FSIT	71PIC/LED
88AND/PAT		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED
89VES/BAR	N	298.1–318.1	5	0.50	not specified		C_p	BSAO	79VES/ZAB

79GRI/YAN data above 385.43 K measured at elevated pressures up to 0.74 MPa
89VES/BAR *water content* 0.04 *mass %*

TABLE 42.41.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
29KEL2	229.6–290.0	7	1.00	0.832	2.24–1	0.83	2.89–2	–3
79GRI/YAN	303.7–462.0	9	0.90	0.549	1.78–1	0.49	6.59–2	3
83BEN/DAR	298.1	1	0.30	0.300	2.60–2	0.09	2.60–2	1
84BRA/PIN	298.1	1	0.30#	1.132	9.79–2	0.34	–9.79–2	–1
85COS/PAT8	283.1–313.1	3	0.30	1.492	1.35–1	0.45	–1.11–1	–3
86TAN/TOY	298.1	1	0.30	0.189	1.64–2	0.06	1.64–2	1
88AND/PAT	298.1	1	0.30#	1.224	1.07–1	0.37	1.07–1	1
89VES/BAR	298.1–318.1	5	0.50	1.055	1.56–1	0.53	1.16–1	3
				Rejected data				
59HUT/BAI	(3.19–1, 1.09, 3.19–1, 1)			73KAL/WOY	(3.54–1, 1.18, 3.54–1, 1)			
81ARU	(4.77–1, 1.31,–1.02–1, –2)			84KAL/WOY	(1.13, 4.28, 1.13, 34)			
86ORT	(3.11–1, 1.09,–3.11–1, –1)							

TABLE 42.41.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	72	28	1.016	1.95–1	0.65	3.91–2	2
C_{sat}	72	28	1.017	1.95–1	0.65	3.91–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
229.6–290.0	2.59720+1	–1.56310	–1.90878	9.27316–1	IV
290.0–360.0	1.89249+2	–1.70470+2	5.63350+1	–5.76738	IV
360.0–462.0	–1.26316+2	9.25005+1	–1.67124+1	9.96273–1	IV
229.6–290.0	2.57138+1	–1.27398	–2.01608	9.40522–1	IV
290.0–360.0	1.89581+2	–1.70791+2	5.64382+1	–5.77836	IV
360.0–462.0	–1.23803+2	9.03614+1	–1.61042+1	9.38534–1	IV

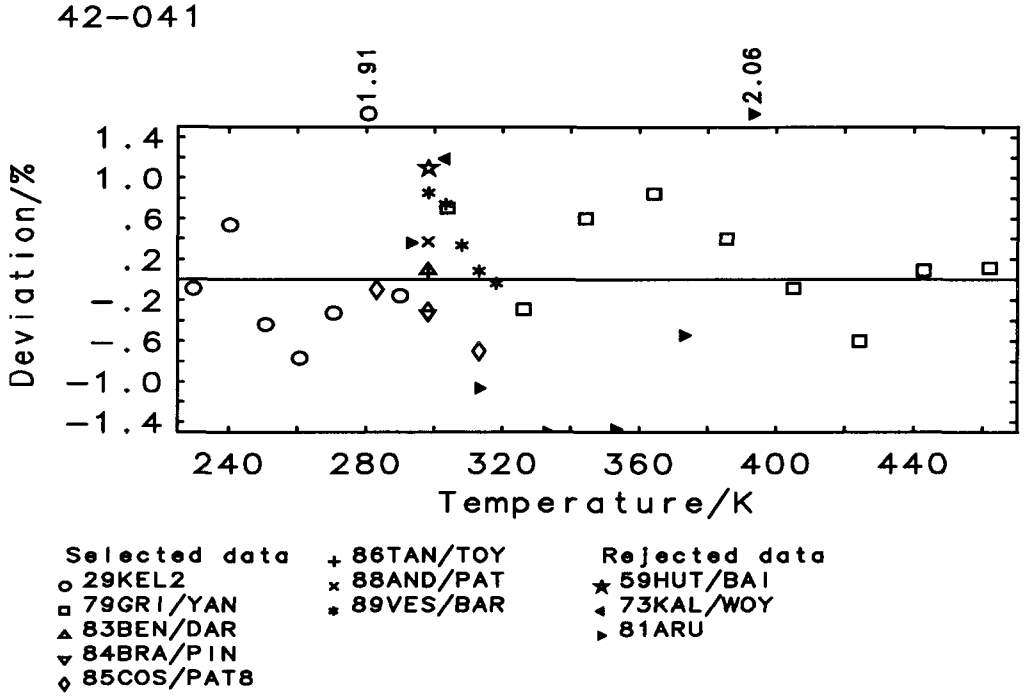
TABLE 42.41.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.917	1.957	2.004	2.059	2.123	2.145	2.196
C_p (J K^{-1}mol^{-1})	195.9	199.9	204.7	210.4	216.9	219.2	224.4
c_{sat} (J K^{-1}g^{-1})	1.917	1.957	2.004	2.059	2.123	2.145	2.196
C_{sat} (J K^{-1}mol^{-1})	195.9	199.9	204.7	210.4	216.9	219.2	224.4
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.279	2.353	2.371	2.470	2.574	2.679	2.783
C_p (J K^{-1}mol^{-1})	232.8	240.4	242.2	252.4	263.0	273.7	284.4
c_{sat} (J K^{-1}g^{-1})	2.279	2.353	2.371	2.470	2.574	2.679	2.783
C_{sat} (J K^{-1}mol^{-1})	232.8	240.4	242.2	252.4	263.0	273.7	284.4
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.883	2.976	3.060	3.135	3.201	3.259	3.309
C_p (J K^{-1}mol^{-1})	294.6	304.1	312.7	320.3	327.1	333.0	338.1
c_{sat} (J K^{-1}g^{-1})	2.883	2.976	3.060	3.135	3.201	3.258	3.308
C_{sat} (J K^{-1}mol^{-1})	294.6	304.1	312.7	320.3	327.0	332.9	338.0
Temp. (K)	420	430	440	450	460		
c_p (J K^{-1}g^{-1})	3.352	3.388	3.418	3.442	3.460		
C_p (J K^{-1}mol^{-1})	342.5	346.2	349.2	351.7	353.6		
c_{sat} (J K^{-1}g^{-1})	3.350	3.385	3.414	3.437	3.454		
C_{sat} (J K^{-1}mol^{-1})	342.3	345.9	348.9	351.2	352.9		

TABLE 42.41.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	72	28	1.127	2.79–1	0.81	3.32–2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
229.6–462.0	610.70	3.72758+3	3.81644+2	–3.92850+2	3.72789+3	–7.63399–1	3.03450+3	IV



Name: 2–Hexanol
Formula: $C_6H_{14}O$

CAS–RN: 626–93–7
Group No.: 42–042
Molar Mass: 102.18

TABLE 42.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
59HUT/BAI	298.1	1	nosp	not specified		C_p	BSIO	55HUT/MAN
86ORT	298.1	1	1.00	98.	anal	C_p	BDCT	70PAZ/PAZ
88TAN/LUO	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 42.42.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88TAN/LUO	298.1	1	0.50#	0.000	0.00	0.00	0.00	0
				Rejected data				
59HUT/BAI	(1.19, 4.01,–1.19, –1)		86ORT	(4.85–1, 1.55, 4.85–1, 1)				

TABLE 42.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		3.08268+1					IV

TABLE 42.42.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J $K^{-1}g^{-1}$)	2.509
C_p (J $K^{-1}mol^{-1}$)	256.3

Name: 3–Hexanol
Formula: $C_6H_{14}O$

CAS–RN: 623–37–0
Group No.: 42–043
Molar Mass: 102.18

TABLE 42.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
88TAN/LUO	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 42.43.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88TAN/LUO	298.1	1	0.50#	0.000	0.00	0.00	0.00	0
				Rejected data				
76CON/GIA	(2.03, 5.91, 2.03, 1)							

TABLE 42.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		3.23856+1					IV

TABLE 42.43.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J $K^{-1}g^{-1}$)	2.635
C_p (J $K^{-1}mol^{-1}$)	269.3

Name: 2–Methyl–1–pentanol
Formula: $C_6H_{14}O$

CAS–RN: 105–30–6
Group No.: 42–044
Molar Mass: 102.18

TABLE 42.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79MAR/BRA	298.1	1	1.00	not specified		C_p	BDCT	70PAZ/PAZ
83AIC/KUM	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
84BRA/PIN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
85BEN/DAR	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 42.44.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79MAR/BRA	298.1	1	1.00	0.311	9.33–2	0.31	9.33–2	1
83AIC/KUM	298.1	1	0.30	0.044	3.98–3	0.01	–3.98–3	–1
84BRA/PIN	298.1	1	0.30	1.081	9.66–2	0.32	–9.66–2	–1
85BEN/DAR	298.1	1	0.30	1.039	9.34–2	0.31	9.34–2	1

TABLE 42.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.885	9.45–2	0.32	2.15–2	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.98795+1	III

TABLE 42.44.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.431
C_p (J K^{-1}mol^{-1})	248.4

Name: 2–Methyl–2–pentanol
Formula: $C_6H_{14}O$

CAS–RN: 590–36–3
Group No.: 42–045
Molar Mass: 102.18

TABLE 42.45.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86ORT	298.15	2.829	1.00	98.	anal	C_p	BDCT	70PAZ/PAZ

Name: 3–Methyl–2–pentanol
Formula: $C_6H_{14}O$

CAS–RN: 565–60–6
Group No.: 42–046
Molar Mass: 102.18

TABLE 42.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79MAR/BRA	298.1	1	1.00	not specified		C_p	BDCT	70PAZ/PAZ
84BRA/PIN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 42.46.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79MAR/BRA	298.1	1	1.00	0.165	5.49–2	0.17	5.49–2	1
84BRA/PIN	298.1	1	0.30	0.049	4.93–3	0.01	–4.93–3	–1

TABLE 42.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.172	5.51–2	0.17	2.50–2	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.31867+1	IV

TABLE 42.46.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.701
C_p (J K^{-1}mol^{-1})	275.9

Name: 3–Methyl–3–pentanol
Formula: $C_6H_{14}O$

CAS–RN: 77–74–7
Group No.: 42–047
Molar Mass: 102.18

TABLE 42.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79MAR/BRA	298.1	1	1.00	not specified		C_p	BDCT	70PAZ/PAZ
84BRA/PIN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
86ORT	298.1	1	1.00	98.	anal	C_p	BDCT	70PAZ/PAZ
88CAC/COS	283.1–323.1	4	nosp	not specified		C_p	FSIT	71PIC/LED

TABLE 42.47.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79MAR/BRA	298.1	1	1.00	0.912	3.28–1	0.91	3.28–1	1
84BRA/PIN	298.1	1	0.30	3.827	4.05–1	1.15	–4.05–1	–1
86ORT	298.1	1	1.00	0.993	3.51–1	0.99	–3.51–1	–1
88CAC/COS	283.1–323.1	4	0.50#	2.065	3.74–1	1.03	2.99–1	4

TABLE 42.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	2.589	4.37–1	1.22	1.09–1	3
Temp. range K		A_1	A_2				Level of uncertainty
283.1–323.1		–1.54567+1	1.71549+1				IV

TABLE 42.47.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.651	2.791	2.904	2.930	3.070	3.209
C_p (J K^{-1}mol^{-1})	270.9	285.1	296.7	299.4	313.7	327.9

Name: 4–Methyl–2–pentanol
Formula: $C_6H_{14}O$

CAS–RN: 108–11–2
Group No.: 42–048
Molar Mass: 102.18

TABLE 42.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84BRA/PIN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
86ORT	298.1	1	1.00	98.	anal	C_p	BDCT	70PAZ/PAZ

TABLE 42.48.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
84BRA/PIN	298.1	1	0.30	0.068	6.68–3	0.02	6.68–3	1
86ORT	298.1	1	1.00	0.226	7.39–2	0.23	–7.39–2	–1

TABLE 42.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.236	7.42–2	0.23	–3.36–2	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		3.28287+1					IV

TABLE 42.48.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.671
C_p (J K^{-1}mol^{-1})	273.0

Name: 2–Ethyl–2–(hydroxymethyl)–1,3–propanediol
Formula: $C_6H_{14}O_3$

CAS–RN: 77–99–6
Group No.: 42–049
Molar Mass: 134.18

TABLE 42.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
89ZHA/YAN2	339.7–354.2	4	nosp	99.12	melpt	C_p	BSAO	88ZHA/ZOU

TABLE 42.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.117	4.98–1	1.12	5.53–3	0
Temp. range K		A_1	A_2				Level of uncertainty
339.7–354.2		1.49032+1	8.57633				IV

TABLE 42.49.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p (J K^{-1}g^{-1})	2.730	2.784
C_p (J K^{-1}mol^{-1})	366.4	373.5

Name: *D*–Mannitol
Formula: $C_6H_{14}O_6$

CAS–RN: 69–65–8
Group No.: 42–050
Molar Mass: 182.17

TABLE 42.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
32SPA/THO	N	453.1–473.1	3S	1.00	not specified		C_p	BDHO	31THO/PAR

32SPA/THO unspecified chirality; indicated n.m.t. corresponds to *D*–Mannitol

TABLE 42.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.057	3.74–2	0.06	1.27–5	1
Temp. range K		A_1	A_2				Level of uncertainty
453.1–473.1		5.97609+1	1.37445				V

TABLE 42.50.4. Recommended values of heat capacities

Temp. (K)	450	460	470
c_p ($J K^{-1} g^{-1}$)	3.01	3.02	3.02
C_p ($J K^{-1} mol^{-1}$)	548	549	551

Name: Benzenemethanol
Formula: C_7H_8O

CAS–RN: 100–51–6
Group No.: 42–051
Molar Mass: 108.14

TABLE 42.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		323.0–391.7	5S	nosp	not specified		C_{avg}	DSIO	*81VON
*98LOU	N	384.1	1	nosp	not specified		C_{avg}	DSIO	*98LOU
02LOU1	N	380.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
31SMI/AND1		259.8–298.5	4	nosp	99.	estim	C_p	DSIO	26AND/LYN
36PAR/TOD1		260.0–300.0	5S	0.70	not specified		C_p	BSIO	25PAR
47SKU		293.1	1	0.30	not specified		C_p	BSAO	47SKU
75NIC/WAD		298.1	1	nosp	99.5	chrom	C_p	BSIO	70LKB/COM
79GRI/YAN		307.5–461.7	9	0.90	not specified		C_p	BDAO	75RAS/GRI
86KRU/FED		373.1	1	nosp	not specified		C_p	BDHT	68OST/DOB

*98LOU average value in temperature range 295–473 K
02LOU1 average value in temperature range 293–468 K

TABLE 42.51.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
02LOU1	380.6	1	3.00#	0.085	7.70–2	0.25	7.70–2	1
31SMI/AND1	259.8–298.5	4	2.00#	0.295	1.39–1	0.59	–1.21–1	–4
36PAR/TOD1	260.0–300.0	5	0.70	0.482	8.74–2	0.34	6.19–2	4
75NIC/WAD	298.1	1	0.30#	1.064	8.29–2	0.32	–8.29–2	–1
79GRI/YAN	307.5–461.7	9	0.90	0.440	1.11–1	0.40	3.84–2	5
				Rejected data				
*81VON	(9.48–1, 3.25,–8.36–1, –5)			*98LOU	(1.01, 3.45,–1.01, –1)			
47SKU	(4.70–1, 1.79, 4.70–1, 1)			86KRU/FED	(2.19, 7.87,–2.19, –1)			

TABLE 42.51.3. Parameters of regression polynomial

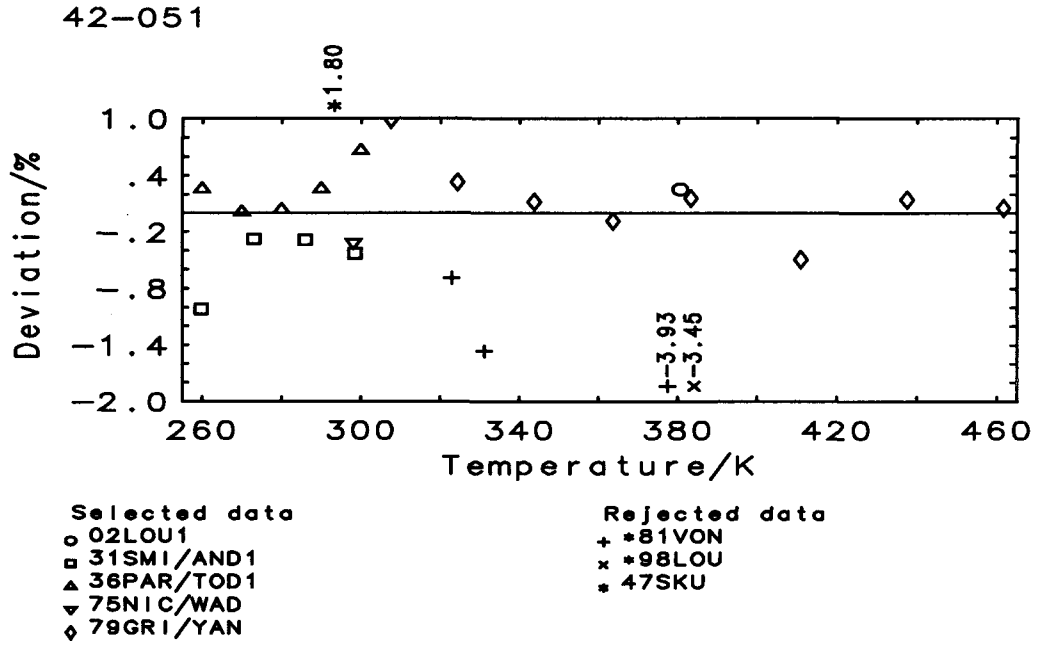
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	20	0.524	1.22–1	0.47	8.16–3	5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
259.8–461.7		–2.94009+1	3.46267+1	–6.81322	4.82227–1		IV

TABLE 42.51.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.772	1.839	1.859	1.901	1.959	2.003	2.013
C_p (J K^{-1}mol^{-1})	191.6	198.8	201.0	205.6	211.8	216.6	217.7
Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.063	2.110	2.153	2.193	2.230	2.265	2.297
C_p (J K^{-1}mol^{-1})	223.1	228.1	232.8	237.2	241.2	244.9	248.4
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.326	2.354	2.380	2.405	2.428	2.449	2.470
C_p (J K^{-1}mol^{-1})	251.6	254.6	257.4	260.0	262.5	264.9	267.2
Temp. (K)	450	460					
c_p (J K^{-1}g^{-1})	2.491	2.511					
C_p (J K^{-1}mol^{-1})	269.3	271.5					

TABLE 42.51.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	20	0.990	2.47–1	0.95	–1.19–1	–11
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
259.8–461.7	677.00	8.40217+1	1.10042+1	–1.53877+1	1.60386+2		IV



Name: 2-Methylphenol
Formula: C_7H_8O

CAS-RN: 95-48-7
Group No.: 42-052
Molar Mass: 108.14

TABLE 42.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
16BRA	283.1	1	nosp	not specified	C_{avg}	DSTO	16BRA
67AND/COU	304.2-400.0	11S	0.10	99.97 melpt	C_p	BSAO	67AND/COU
67RAS/GAN	313.1-373.1	4S	0.50	not specified	C_p	BSAO	67RAS/GAN
90MEV/LIC	304.0	1	3.00	99. anal	C_p	BDCT	89BRE/LIC

TABLE 42.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
67AND/COU	304.2-400.0	11	0.10	0.261	7.58-3	0.03	2.60-6	0
				Rejected data				
67RAS/GAN	(3.07-1, 1.06,-3.01-1, -4)							

TABLE 42.52.3. Parameters of regression polynomial

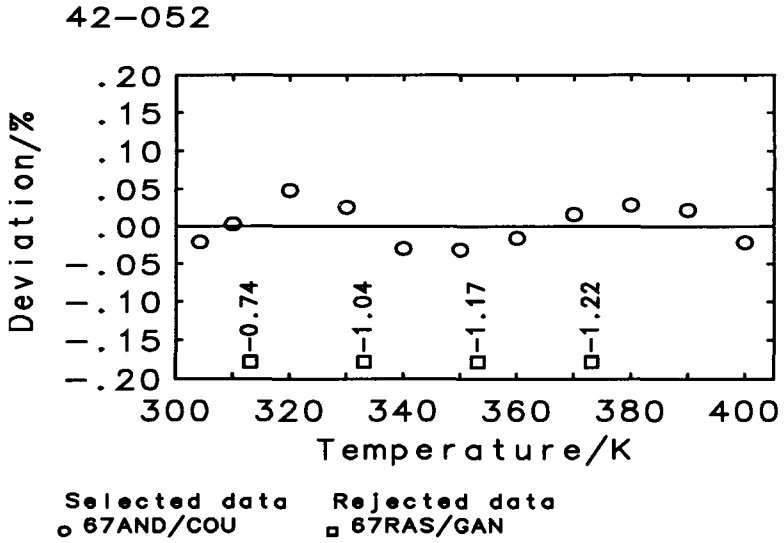
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	17	11	0.326	9.50-3	0.03	2.60-6	0
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
304.2-400.0	-2.26831+1	3.82228+1	-9.77006	8.82407-1			III

TABLE 42.52.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	2.169	2.191	2.212	2.231	2.249	2.266	2.282
C_p ($J K^{-1}mol^{-1}$)	234.5	237.0	239.2	241.2	243.2	245.0	246.8
Temp. (K)	380	390	400				
c_p ($J K^{-1}g^{-1}$)	2.299	2.316	2.334				
C_p ($J K^{-1}mol^{-1}$)	248.6	250.5	252.4				

TABLE 42.52.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	17	11	0.837	2.42-2	0.08	2.84-5	-1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
304.2-400.0	697.55	1.82904+1	1.80659	1.51320+1	4.62942+1		III



Name: 3–Methylphenol
Formula: C_7H_8O

CAS–RN: 108–39–4
Group No.: 42–053
Molar Mass: 108.14

TABLE 42.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
00LOU	N	382.1	1	nosp	not specified	C_{avg}	DSIO	*98LOU
16BRA		283.1	1	nosp	not specified	C_{avg}	DSTO	16BRA
51TSC/KRI		298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
67AND/COU	N	285.4–400.0	14S	0.10	99.89 melpt	C_p	BSAO	67AND/COU
67RAS/GAN		293.1–373.1	5S	0.50	not specified	C_p	BSAO	67RAS/GAN
90MEV/LIC		280.8	1	3.00	99. anal	C_p	BDCT	89BRE/LIC

00LOU average value in temperature range 294–470 K
67AND/COU data up to 300 K measured with adiabatic calorimeter 63AND/CON

TABLE 42.53.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67AND/COU	285.4–400.0	14	0.10	0.101	2.86–3	0.01	4.90–6	1
				Rejected data				
00LOU	(1.57–1, 0.52,–1.57–1, –1)			51TSC/KRI	(7.16–1, 2.72,–7.16–1, –1)			
67RAS/GAN	(3.29–1, 1.17,–3.05–1, –5)							

TABLE 42.53.3. Parameters of regression polynomial

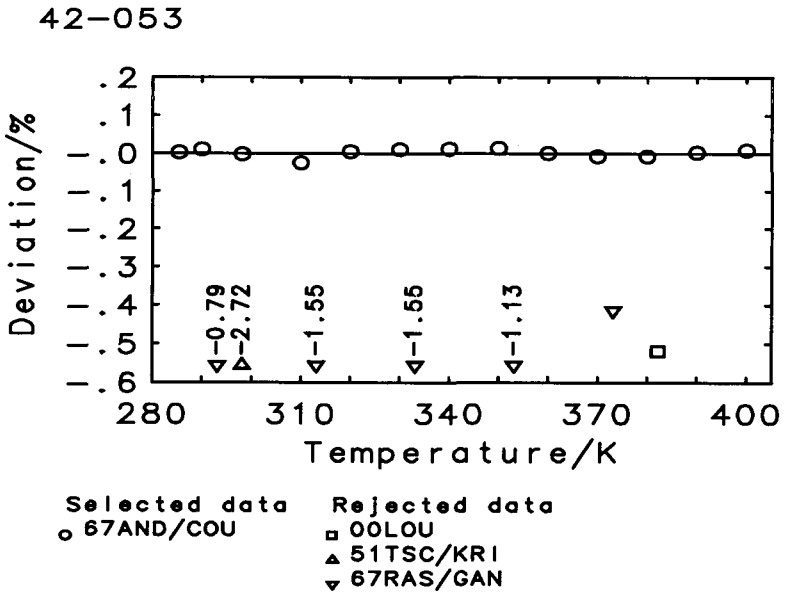
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	14	0.120	3.38–3	0.01	4.90–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
285.4–400.0		–2.86617+1	3.82776+1	–8.66399	7.02107–1		II

TABLE 42.53.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	2.045	2.080	2.088	2.126	2.162	2.194	2.224
C_p ($J K^{-1} mol^{-1}$)	221.2	224.9	225.8	229.9	233.8	237.3	240.5
Temp. (K)	350	360	370	380	390	400	
c_p ($J K^{-1} g^{-1}$)	2.251	2.277	2.300	2.323	2.344	2.365	
C_p ($J K^{-1} mol^{-1}$)	243.4	246.2	248.8	251.2	253.5	255.8	

TABLE 42.53.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	14	1.039	3.01–2	0.10	4.17–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
285.4–400.0	705.75	9.48950+1	1.43143+1	–1.20910+1	1.57273+2		II



Name: 4–Methylphenol
Formula: C_7H_8O

CAS–RN: 106–44–5
Group No.: 42–054
Molar Mass: 108.14

TABLE 42.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67AND/COU	307.9–400.0	11S	0.10	99.98	melpt	C_p	BSAO	67AND/COU
67RAS/GAN	313.1–373.1	4S	0.50	not specified		C_p	BSAO	67RAS/GAN
75NIC/WAD	298.1	1	nosp	99.5	chrom	C_p	BSIO	70LKB/COM
90MEV/LIC	313.0–353.0	eqn	3.00	99.	anal	C_p	BDCT	89BRE/LIC

TABLE 42.54.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67AND/COU	307.9–400.0	11	0.10	0.313	9.20–3	0.03	7.28–6	2
				Rejected data				
67RAS/GAN	(4.53–1, 1.59,–4.51–1, –4)			90MEV/LIC	(7.86–1, 2.71, 7.15–1, 5)			

TABLE 42.54.3. Parameters of regression polynomial

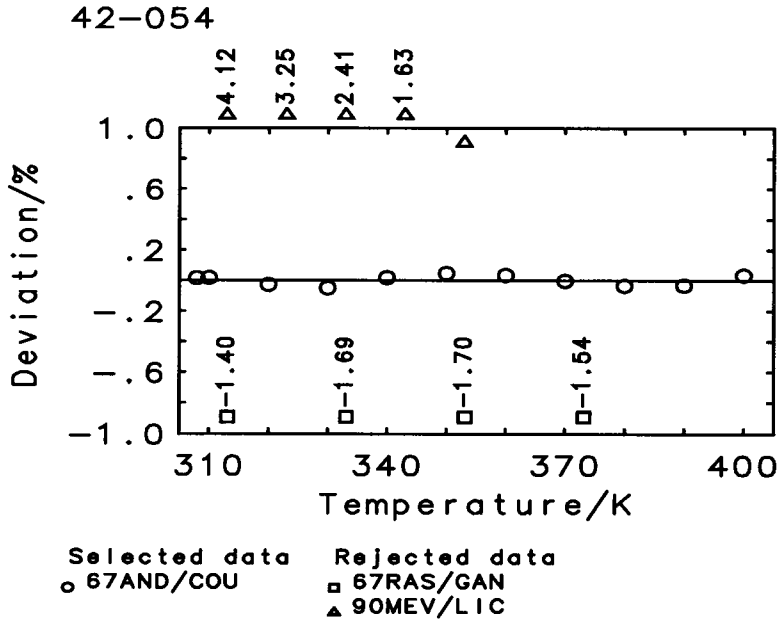
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	11	0.392	1.15–2	0.04	7.28–6	2
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
307.9–400.0	3.23809+1	–1.43392+1	6.22047	–6.80135–1			II

TABLE 42.54.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	2.110	2.146	2.181	2.215	2.248	2.279	2.309
C_p ($J K^{-1} mol^{-1}$)	228.2	232.0	235.8	239.5	243.1	246.5	249.7
Temp. (K)	380	390	400				
c_p ($J K^{-1} g^{-1}$)	2.337	2.362	2.385				
C_p ($J K^{-1} mol^{-1}$)	252.7	255.5	257.9				

TABLE 42.54.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	11	0.563	1.61–2	0.06	1.79–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
307.9–400.0	704.55	4.45539+1	5.09256	1.30247	9.74485+1		II



Name: Cycloheptanol
Formula: $C_7H_{14}O$

CAS-RN: 502–41–0
Group No.: 42–055
Molar Mass: 114.19

TABLE 42.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72ADA/SUG	283.2–316.1	8	nosp	99.932	melpt	C_p	BSAO	65SUG/SEK
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA

TABLE 42.55.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
72ADA/SUG	283.2–316.1	8	0.20#	0.192	1.19–2	0.04	2.57–5	0
				Rejected data				
76CON/GIA	(7.09–1, 2.41,–7.09–1, –1)							

TABLE 42.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	8	0.221	1.37–2	0.04	2.57–5	0
Temp. range K		A_1	A_2				Level of uncertainty
283.2–316.1		−1.12723+1	1.38752+1				II

TABLE 42.55.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	2.008	2.109	2.191	2.210	2.311	2.412
C_p ($J K^{-1}mol^{-1}$)	229.3	240.8	250.2	252.4	263.9	275.4

Name: 1–Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS–RN: 590–67–0
Group No.: 42–056
Molar Mass: 114.19

TABLE 42.56.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	2.444	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 2–Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS–RN: 583–59–5
Group No.: 42–057
Molar Mass: 114.19

TABLE 42.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	N	289.6	1	nosp	not specified		C_p	DSIO	22HER/SCH
88CAC/COS		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED

24HER/BLO probably racemic *trans*–isomer (according to n.b.t. and refractive index)

TABLE 42.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88CAC/COS	298.1	1	0.50#	0.000	0.00	0.00	0.00	0

TABLE 42.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.21655+1	IV

TABLE 42.57.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1}g^{-1}$)	2.342
C_p ($J K^{-1}mol^{-1}$)	267.4

Name: *cis*–2–Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS–RN: 7443–70–1
Group No.: 42–058
Molar Mass: 114.19

TABLE 42.58.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	2.355	nosp	not specified		C_p	FSIT	71PIC/LED

Name: *trans*–2–Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS–RN: 7443–52–9
Group No.: 42–059
Molar Mass: 114.19

TABLE 42.59.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	2.303	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 3–Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS–RN: 591–23–1
Group No.: 42–060
Molar Mass: 114.19

TABLE 42.60.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.65	1.766	nosp	not specified		C_p	DSIO	22HER/SCH

Name: 4–Methylcyclohexanol
Formula: $C_7H_{14}O$

CAS–RN: 589–91–3
Group No.: 42–061
Molar Mass: 114.19

TABLE 42.61.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.65	1.770	nosp	not specified		C_p	DSIO	22HER/SCH

Name: 3–Ethyl–3–pentanol
Formula: $C_7H_{16}O$

CAS–RN: 597–49–9
Group No.: 42–062
Molar Mass: 116.20

TABLE 42.62.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	3.046	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 1–Heptanol
Formula: $C_7H_{16}O$

CAS–RN: 111–70–6
Group No.: 42–063
Molar Mass: 116.20

TABLE 42.63.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
56PAR/KEN		240.0–300.0	7S	1.00	98.2	melpt	C_p	BSIO	25PAR
59HUT/BAI		298.1	1	nosp	not specified		C_p	BSIO	55HUT/MAN
67GRA		308.1–338.1	4	1.00	not specified		C_p	BSIO	67GRA
79GRI/YAN	N	303.0–462.3	9	0.90	not specified		C_p	BDAO	75RAS/GRI
80VAS/TRE		323.0–453.0	eqn	2.00	99.8	anal	C_{sat}	BSAO	80VAS/TRE
88AND/PAT		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED
88NAZ/BAS		303.4–447.1	7	2.20	99.2	anal	C_p	BDHO	86NAZ/BAS1
89VES/BAR	N	298.1–318.1	5	0.50	not specified		C_p	BSAO	79VES/ZAB

79GRI/YAN data above 425.19 K were measured at elevated pressures up to 0.27 MPa
89VES/BAR water content 0.007 mass %

TABLE 42.63.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56PAR/KEN	240.0–300.0	7	1.00	1.190	3.87–1	1.19	1.51–1	1
59HUT/BAI	298.1	1	0.50#	0.808	1.33–1	0.40	1.33–1	1
79GRI/YAN	303.0–462.3	9	0.90	0.458	1.61–1	0.41	7.75–2	5
88AND/PAT	298.1	1	0.30#	0.218	2.15–2	0.07	2.15–2	1
89VES/BAR	298.1–318.1	5	0.50	0.808	1.38–1	0.40	–1.29–1	–5
				Rejected data				
67GRA	(8.64–1, 2.48,–8.56–1, –4)			80VAS/TRE	(9.93–1, 2.45,–9.47–1, –10)			
88NAZ/BAS	(1.43, 3.73, 1.83–1, 1)							

TABLE 42.63.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	44	23	0.963	2.87–1	0.85	5.51–2	3
C_{sat}	44	23	0.963	2.87–1	0.86	5.51–2	3

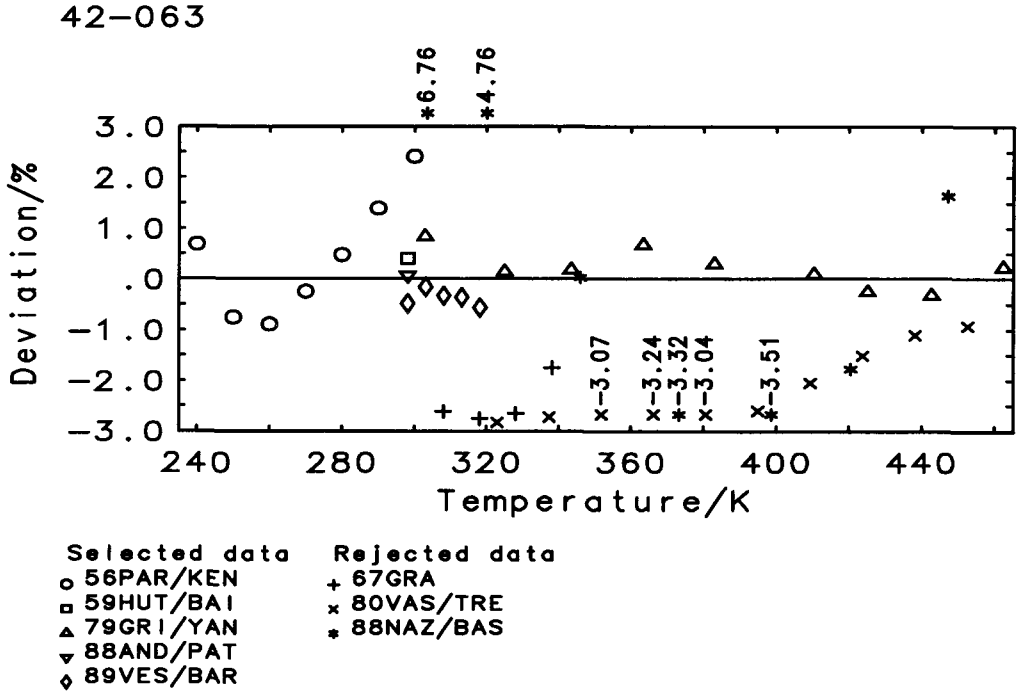
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
240.0–300.0	–2.33933+2	2.82767+2	–1.03214+2	1.28698+1	IV
300.0–360.0	4.55124+2	–4.06290+2	1.26472+2	–1.26508+1	IV
360.0–462.3	–2.77519+2	2.04246+2	–4.31216+1	3.05225	V
240.0–300.0	–2.34084+2	2.82931+2	–1.03273+2	1.28769+1	IV
300.0–360.0	4.55373+2	–4.06526+2	1.26546+2	–1.26586+1	IV
360.0–462.3	–2.75784+2	2.02772+2	–4.27037+1	3.01269	V

TABLE 42.63.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	2.011	2.074	2.127	2.177	2.192	2.228	2.286
C_p ($J K^{-1}mol^{-1}$)	233.7	241.0	247.2	253.0	254.8	258.9	265.6
c_{sat} ($J K^{-1}g^{-1}$)	2.011	2.074	2.127	2.177	2.192	2.228	2.286
C_{sat} ($J K^{-1}mol^{-1}$)	233.7	241.0	247.2	253.0	254.8	258.9	265.6
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	2.342	2.356	2.442	2.542	2.648	2.756	2.861
C_p ($J K^{-1}mol^{-1}$)	272.1	273.8	283.8	295.4	307.7	320.3	332.4
c_{sat} ($J K^{-1}g^{-1}$)	2.342	2.356	2.442	2.542	2.648	2.756	2.861
C_{sat} ($J K^{-1}mol^{-1}$)	272.1	273.8	283.8	295.4	307.7	320.3	332.4
Temp. (K)	360	370	380	390	400	410	420
c_p ($J K^{-1}g^{-1}$)	2.956	3.04	3.11	3.16	3.21	3.25	3.28
C_p ($J K^{-1}mol^{-1}$)	343.5	353	361	368	373	377	381
c_{sat} ($J K^{-1}g^{-1}$)	2.956	3.04	3.11	3.16	3.21	3.25	3.27
C_{sat} ($J K^{-1}mol^{-1}$)	343.5	353	361	368	373	377	381
Temp. (K)	430	440	450	460			
c_p ($J K^{-1}g^{-1}$)	3.30	3.31	3.33	3.34			
C_p ($J K^{-1}mol^{-1}$)	383	385	387	388			
c_{sat} ($J K^{-1}g^{-1}$)	3.30	3.31	3.33	3.33			
C_{sat} ($J K^{-1}mol^{-1}$)	383	385	386	387			

TABLE 42.63.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	44	23	1.565	3.12–1	0.91	–5.82–2	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
240.0–462.3	632.50	6.59046+3	7.15941+2	–7.42462+2	6.46917+3	2.86452+2	4.86276+3	V



Name: 2–Heptanol
Formula: $C_7H_{16}O$

CAS–RN: 543–49–7
Group No.: 42–064
Molar Mass: 116.20

TABLE 42.64.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59HUT/BAI	298.15	2.366	nosp	not specified		C_p	BSIO	55HUT/MAN

Name: 4–Heptanol
Formula: $C_7H_{16}O$

CAS–RN: 589–55–9
Group No.: 42–065
Molar Mass: 116.20

TABLE 42.65.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CON/GIA	298.15	2.733	nosp	not specified		C_p	BDCT	76CON/GIA

Name: Benzeneethanol
Formula: $C_8H_{10}O$

CAS–RN: 60–12–8
Group No.: 42–066
Molar Mass: 122.17

TABLE 42.66.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75NIC/WAD	298.15	2.068	nosp	99.5	chrom	C_p	BSIO	70LKB/COM

Name: 2–Ethyl–1–hexanol
Formula: $C_8H_{18}O$

CAS–RN: 104–76–7
Group No.: 42–067
Molar Mass: 130.23

TABLE 42.67.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
58ANO	298.1	1	nosp	not specified		C_p	not specified	
78RYB/EME	293.1–353.1	7S	nosp	not specified		C_p	BSIO	78RYB/EME

TABLE 42.67.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
78RYB/EME	293.1–353.1	7	2.00#	0.005	3.88–3	0.01	8.72–6	0
				Rejected data				
58ANO	(1.68, 4.53,–1.68, –1)							

TABLE 42.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.005	4.59–3	0.01	8.72–6	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–353.1		–6.73290	1.52258+1				V

TABLE 42.67.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.39	2.47	2.49	2.58	2.68	2.78	2.88
C_p (J K^{-1}mol^{-1})	311	321	324	336	349	362	374
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	2.97						
C_p (J K^{-1}mol^{-1})	387						

Name: 2–Methyl–1–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 106–67–2
Group No.: 42–068
Molar Mass: 130.23

TABLE 42.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31CLI/AND	259.8–310.7	5	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.062	6.64–2	0.19	7.55–5	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
259.8–310.7		1.96907+2	–1.26170+2	2.43877+1			V

TABLE 42.68.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.15	2.17	2.19	2.22	2.31	2.40	2.42
C_p (J K^{-1}mol^{-1})	280	283	285	290	300	312	315
Temp. (K)	310						
c_p (J K^{-1}g^{-1})	2.56						
C_p (J K^{-1}mol^{-1})	334						

Name: 2–Methyl–2–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 625–25–2
Group No.: 42–069
Molar Mass: 130.23

TABLE 42.69.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	231.7–310.7	7	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.254	2.54–1	0.76	4.27–3	–1

Temp. range K	A_1	A_2	Level of uncertainty
231.7–310.7	–1.44422	1.40427+1	V

TABLE 42.69.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J\,K^{-1}g^{-1}$)	1.97	2.06	2.15	2.24	2.33	2.36	2.42
C_p ($J\,K^{-1}mol^{-1}$)	257	268	280	292	303	307	315

Temp. (K)	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	2.51	2.58	2.60	2.69
C_p ($J\,K^{-1}mol^{-1}$)	327	336	338	350

Name: 2–Methyl–4–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 21570–35–4
Group No.: 42–070
Molar Mass: 130.23

TABLE 42.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	201.1–298.5	8	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.071	6.81–2	0.21	1.81–5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
201.1–298.5	5.38958+1	–2.80283+1	7.82547	V

TABLE 42.70.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.86	1.89	1.92	1.97	2.02	2.09	2.17
C_p (J K^{-1}mol^{-1})	242	246	250	256	264	272	282
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	2.25	2.28	2.35	2.45	2.55	2.57	
C_p (J K^{-1}mol^{-1})	293	297	306	319	332	335	

Name: 3–Methyl–2–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 31367–46–1
Group No.: 42–071
Molar Mass: 130.23

TABLE 42.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	166.7–298.5	10	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.610	5.75–1	1.83	1.82–2	0
Temp. range K		A_1	A_2				Level of uncertainty
166.7–298.5		1.96449+1	5.48007				V

TABLE 42.71.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.85	1.88	1.92	1.95	1.99	2.02	2.06
C_p (J K^{-1}mol^{-1})	241	245	250	254	259	264	268
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	2.09	2.13	2.16	2.20	2.21	2.23	2.27
C_p (J K^{-1}mol^{-1})	273	277	282	286	288	291	295
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	2.30	2.30					
C_p (J K^{-1}mol^{-1})	299	300					

Name: 4–Methyl–2–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 56298–90–9
Group No.: 42–072
Molar Mass: 130.23

TABLE 42.72.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	184.4–298.5	9	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.72.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.244	2.49–1	0.73	2.27–3	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
184.4–298.5		2.71088+1	–4.96327	2.86668			V

TABLE 42.72.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.75	1.79	1.83	1.87	1.92	1.97	2.02
C_p (J K^{-1}mol^{-1})	228	233	238	244	250	257	264
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.08	2.14	2.21	2.23	2.28	2.35	2.41
C_p (J K^{-1}mol^{-1})	271	279	288	291	297	306	314
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	2.43						
C_p (J K^{-1}mol^{-1})	316						

Name: 4–Methyl–3–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 14979–39–6
Group No.: 42–073
Molar Mass: 130.23

TABLE 42.73.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
31CLI/AND	166.7–298.5	10	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.320	2.92–1	0.96	4.14–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
166.7–298.5		3.90701+1	–1.38651+1	4.43297			V

TABLE 42.73.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.81	1.82	1.83	1.86	1.88	1.92	1.96
C_p (J K^{-1}mol^{-1})	235	237	239	242	245	250	255
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	2.00	2.05	2.11	2.17	2.19	2.23	2.31
C_p (J K^{-1}mol^{-1})	260	267	274	282	285	291	301
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	2.37	2.39					
C_p (J K^{-1}mol^{-1})	309	311					

Name: 4–Methyl–4–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 598–01–6
Group No.: 42–074
Molar Mass: 130.23

TABLE 42.74.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	201.1–298.5	8	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.155	1.84–1	0.46	9.36–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
201.1–298.5		8.06011+1	–5.38474+1	1.39688+1			V

TABLE 42.74.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.84	1.86	1.90	1.96	2.03	2.13	2.24
C_p (J K^{-1}mol^{-1})	239	242	247	255	265	277	291
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	2.37	2.41	2.51	2.68	2.82	2.86	
C_p (J K^{-1}mol^{-1})	308	314	327	349	368	372	

Name: 5–Methyl–1–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 7212–53–5
Group No.: 42–075
Molar Mass: 130.23

TABLE 42.75.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	184.4–298.5	9	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.75.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.213	1.98–1	0.64	1.40–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
184.4–298.5		4.76171+1	–2.17926+1	6.08450			V

TABLE 42.75.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.79	1.80	1.81	1.83	1.86	1.89	1.94
C_p (J K^{-1}mol^{-1})	234	234	236	239	242	247	252
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.99	2.05	2.12	2.14	2.19	2.27	2.34
C_p (J K^{-1}mol^{-1})	259	267	275	278	285	296	305
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	2.36						
C_p (J K^{-1}mol^{-1})	308						

Name: 5–Methyl–2–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 54630–50–1
Group No.: 42–076
Molar Mass: 130.23

TABLE 42.76.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	166.7–298.5	10	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.76.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.365	3.38–1	1.10	5.19–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
166.7–298.5		3.85900+1	–1.36463+1	4.27540			V

TABLE 42.76.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.77	1.78	1.79	1.81	1.84	1.87	1.90
C_p (J K^{-1}mol^{-1})	231	232	234	236	239	243	248
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.95	1.99	2.04	2.10	2.12	2.16	2.23
C_p (J K^{-1}mol^{-1})	253	259	266	274	276	282	291
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	2.29	2.31					
C_p (J K^{-1}mol^{-1})	299	300					

Name: 6–Methyl–2–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 4730–22–7
Group No.: 42–077
Molar Mass: 130.23

TABLE 42.77.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	231.7–298.5	6	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.371	3.57–1	1.11	6.07–3	2
Temp. range K		A_1	A_2				Level of uncertainty
231.7–298.5		6.50129	1.04962+1				V

TABLE 42.77.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.96	2.02	2.09	2.16	2.22	2.25	2.29
C_p (J K^{-1}mol^{-1})	255	264	272	281	290	292	298
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	2.36	2.41	2.43				
C_p (J K^{-1}mol^{-1})	307	314	316				

Name: 6–Methyl–3–heptanol
Formula: $C_8H_{18}O$

CAS–RN: 18720–66–6
Group No.: 42–078
Molar Mass: 130.23

TABLE 42.78.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	231.7–322.6	8	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.78.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.206	2.34–1	0.62	2.55–3	0
Temp. range K		A_1	A_2				Level of uncertainty
231.7–322.6		8.08298	9.77028				V

TABLE 42.78.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	1.95	2.01	2.08	2.14	2.20	2.22	2.26
C_p ($J K^{-1} mol^{-1}$)	254	262	270	278	287	289	295
Temp. (K)	290	298.15	300	310	320		
c_p ($J K^{-1} g^{-1}$)	2.33	2.38	2.39	2.45	2.51		
C_p ($J K^{-1} mol^{-1}$)	303	309	311	319	327		

Name: 1–Octanol
Formula: $C_8H_{18}O$

CAS–RN: 111–87–5
Group No.: 42–079
Molar Mass: 130.23

TABLE 42.79.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		314.2–384.8	5S	nosp	not specified		C_{avg}	DSIO	*81VON
31CLI/AND		246.0–286.0	4	nosp	not specified		C_{sat}	DSIO	26AND/LYN
59HUT/BAI		298.1	1	nosp	not specified		C_p	BSIO	55HUT/MAN
61ROU		298.9–311.3	5	nosp	not specified		C_p	BSAO	61ROU
79GRI/YAN		310.7–452.3	8	0.90	not specified		C_p	BDAO	75RAS/GRI
80VAS/TRE		313.0–468.0	eqn	2.00	99.6	anal	C_{sat}	BSAO	80VAS/TRE
86NAZ/BAS2		303.2–448.6	7	2.00	99.6	estim	C_p	BDHO	86NAZ/BAS1
89VES/BAR	N	298.1–318.1	5	0.50	not specified		C_p	BSAO	79VES/ZAB

89VES/BAR water content 0.039 mass %

TABLE 42.79.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31CLI/AND	246.0–286.0	4	2.00#	0.948	5.98–1	1.90	–1.32–1	0
61ROU	298.9–311.3	5	0.50#	1.309	2.44–1	0.65	1.55–1	3
79GRI/YAN	310.7–452.3	8	0.90	0.742	3.14–1	0.67	1.03–1	0
89VES/BAR	298.1–318.1	5	0.50	1.191	2.30–1	0.60	–1.90–1	–3
				Rejected data				
*81VON	(2.81, 6.37,–2.20, –3)			59HUT/BAI	(1.09, 2.89, 1.09, 1)			
80VAS/TRE	(6.22–1, 1.39,–5.90–1, –10)			86NAZ/BAS2	(1.39, 3.18, 1.44–1, –1)			

TABLE 42.79.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	46	22	1.180	4.04–1	1.13	5.61–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
246.0–390.0		1.11517+2	–9.82596+1	3.57913+1	–3.77930		IV
390.0–452.3		–1.95257+2	1.37721+2	–2.47165+1	1.39230		V

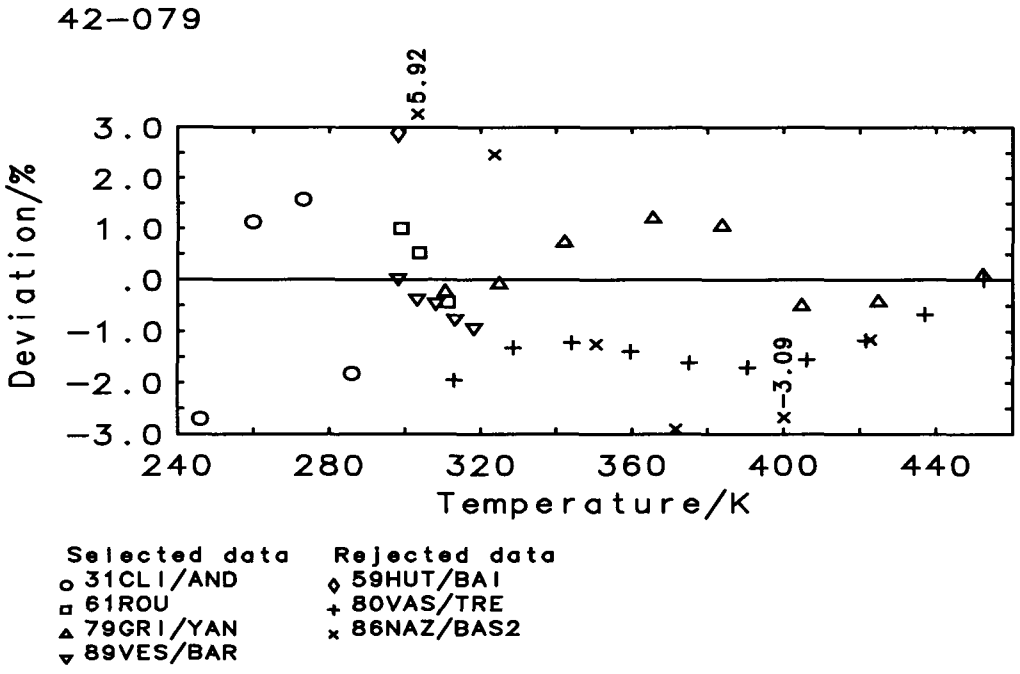
TABLE 42.79.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.948	2.015	2.091	2.116	2.173	2.260	2.334
C_p (J K^{-1}mol^{-1})	253.7	262.5	272.3	275.6	283.0	294.3	303.9
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.351	2.444	2.538	2.631	2.722	2.810	2.893
C_p (J K^{-1}mol^{-1})	306.1	318.3	330.5	342.6	354.5	366.0	376.7
Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.969	3.038	3.097	3.15	3.18	3.21	3.23
C_p (J K^{-1}mol^{-1})	386.7	395.6	403.3	410	415	418	421
Temp. (K)	440	450					
c_p (J K^{-1}g^{-1})	3.24	3.25					
C_p (J K^{-1}mol^{-1})	422	423					

TABLE 42.79.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	46	22	1.274	3.82–1	1.05	–7.56–2	–4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
246.0–452.3	652.50	4.54976+3	5.27054+2	–5.08693+2	4.13031+3	1.08864+3	2.49442+3	V



Name: 2–Octanol
Formula: $C_8H_{18}O$

CAS–RN: 123–96–6
Group No.: 42–080
Molar Mass: 130.23

TABLE 42.80.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	246.0–298.5	5	nosp	not specified		C_p	DSIO	26AND/LYN
59HUT/BAI	298.1	1	nosp	not specified		C_p	BSIO	55HUT/MAN
61ROU	298.9–313.7	7	nosp	not specified		C_p	BSAO	61ROU

TABLE 42.80.2. Correlated heat capacities

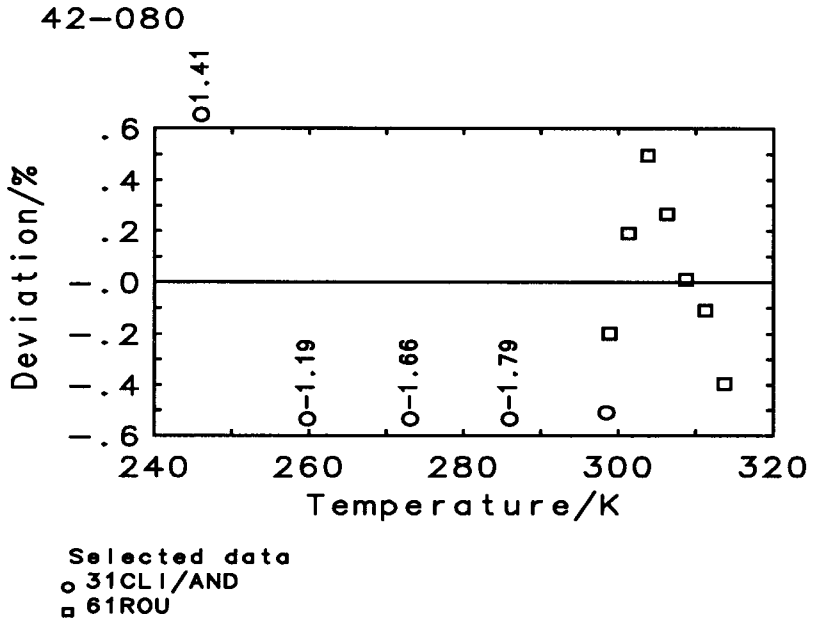
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
31CLI/AND	246.0–298.5	5	2.00#	0.694	4.95–1	1.39	–2.85–1	–3
61ROU	298.9–313.7	7	0.50#	0.566	1.16–1	0.28	1.41–2	0
				Rejected data				
59HUT/BAI	(2.43, 6.48,–2.43, –1)							

TABLE 42.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	12	0.719	3.83–1	1.06	–1.11–1	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
246.0–313.7		–6.11537+1	5.63216+1	–7.52611			V

TABLE 42.80.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J\,K^{-1}g^{-1}$)	2.08	2.20	2.30	2.33	2.40	2.48	2.55
C_p ($J\,K^{-1}mol^{-1}$)	271	286	300	304	312	323	331
Temp. (K)	300	310					
c_p ($J\,K^{-1}g^{-1}$)	2.56	2.63					
C_p ($J\,K^{-1}mol^{-1}$)	333	342					



Name: 3-Octanol
Formula: $C_8H_{18}O$

CAS-RN: 589-98-0
Group No.: 42-081
Molar Mass: 130.23

TABLE 42.81.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	216.9–298.5	7	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.086	8.86-2	0.26	2.39-4	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
216.–298.5		2.73916+1	-3.45020	2.65391			V

TABLE 42.81.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	2.08	2.14	2.20	2.26	2.32	2.39	2.41
C_p (J K^{-1}mol^{-1})	271	278	286	294	302	311	314
Temp. (K)	280	290	298.15	300			
c_p (J K^{-1}g^{-1})	2.46	2.53	2.60	2.61			
C_p (J K^{-1}mol^{-1})	320	330	338	340			

Name: 4–Octanol
Formula: $C_8H_{18}O$

CAS–RN: 589–62–8
Group No.: 42–082
Molar Mass: 130.23

TABLE 42.82.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31CLI/AND	216.9–310.7	8	nosp	not specified		C_p	DSIO	26AND/LYN

TABLE 42.82.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.161	1.67–1	0.48	7.08–4	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
216.9–310.7	4.12408+2	–4.28314+2	1.56983+2	–1.84980+1	V

TABLE 42.82.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	2.10	2.09	2.10	2.15	2.23	2.32	2.35
C_p (J K^{-1}mol^{-1})	274	272	274	280	290	302	306

Temp. (K)	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.41	2.51	2.59	2.61	2.69
C_p (J K^{-1}mol^{-1})	314	327	338	340	351

Name: Benzenepropanol
Formula: $C_9H_{12}O$

CAS–RN: 122–97–4
Group No.: 42–083
Molar Mass: 136.19

TABLE 42.83.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75NIC/WAD	298.15	2.061	nosp	99.5	chrom	C_p	BSIO	70LKB/COM

Name: 1–Nonanol
Formula: $C_9H_{20}O$

CAS–RN: 143–08–8
Group No.: 42–084
Molar Mass: 144.26

TABLE 42.84.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79GRI/YAN	304.2–464.2	10	0.90	not specified		C_p	BDAO	75RAS/GRI
82VAS/PET	303.0–423.0	eqn	nosp	99.2	anal	C_{sat}	BSAO	80VAS/TRE
82VAS/PET	423.0–483.0	eqn	nosp	99.2	anal	C_{sat}	BSAO	80VAS/TRE
86NAZ/BAS2	303.1–474.1	8	2.00	99.4	estim	C_p	BDHO	86NAZ/BAS1

TABLE 42.84.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79GRI/YAN	304.2–464.2	10	0.90	0.214	9.24–2	0.19	3.21–4	2
				Rejected data				
82VAS/PET	(6.14–1, 1.21, 2.45–1, 1)			82VAS/PET	(8.88–1, 1.59, 8.77–1, 5)			
86NAZ/BAS2	(1.52, 3.02,–8.17–1, –2)							

TABLE 42.84.3. Parameters of cubic spline polynomials

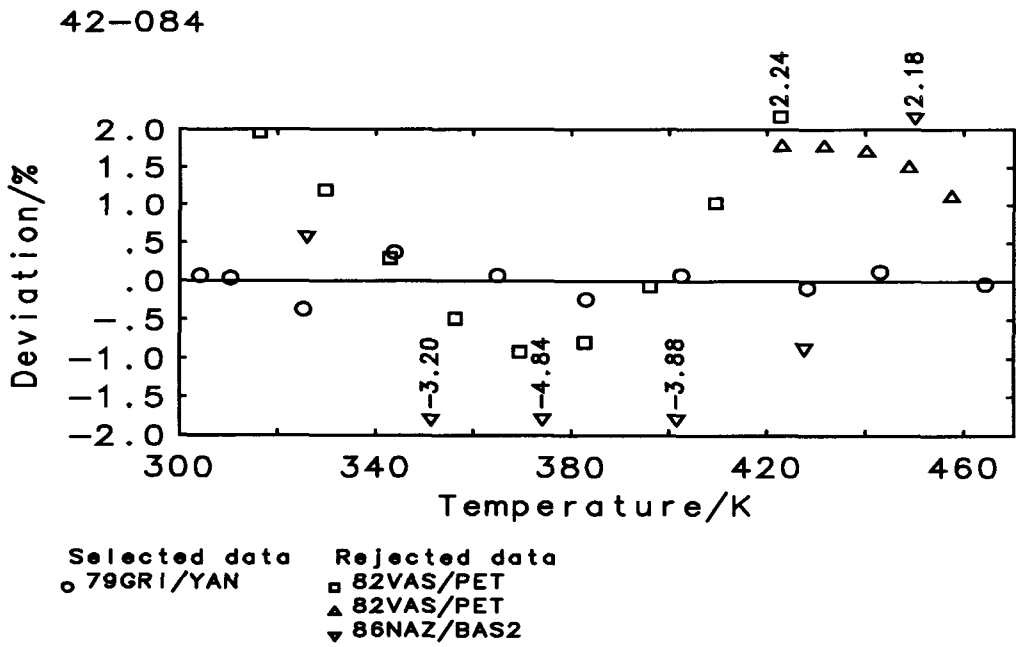
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	36	10	0.303	1.31–1	0.27	3.21–4	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
304.2–380.0		2.95844+2	–2.63852+2	8.58430+1	–8.75247		IV
380.0–464.2		–6.83043+2	5.08953+2	–1.17527+2	9.08700		IV

TABLE 42.84.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	2.338	2.427	2.521	2.618	2.714	2.805	2.890
C_p (J K^{-1}mol^{-1})	337.2	350.1	363.7	377.7	391.5	404.7	416.9
Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.965	3.027	3.073	3.107	3.131	3.148	3.162
C_p (J K^{-1}mol^{-1})	427.7	436.6	443.3	448.2	451.7	454.2	456.2
Temp. (K)	440	450	460				
c_p (J K^{-1}g^{-1})	3.176	3.192	3.214				
C_p (J K^{-1}mol^{-1})	458.1	460.4	463.6				

TABLE 42.84.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	36	10	0.683	3.05–1	0.62	2.84–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
304.2–464.2	671.50	3.84120+2	5.72266+1	–1.23865+2	6.44578+2		IV



Name: 1–Naphthol
Formula: $C_{10}H_8O$

CAS–RN: 90–15–3
Group No.: 42–085
Molar Mass: 144.17

TABLE 42.85.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	368.0–453.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN
67PAC		393.1	1	nosp	not specified		C_p	BDHT	79DU/COM

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 42.85.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
26AND/LYN	368.0–442.2	8	3.00#	0.271	2.81–1	0.81	2.58–1	8
67PAC	393.1	1	1.50#	0.962	4.92–1	1.44	–4.92–1	–1

TABLE 42.85.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	9	0.465	3.53–1	1.03	1.75–1	7

Temp. range K	A_1	A_2	Level of uncertainty
368.0–442.2	1.10284+1	5.99315	V

TABLE 42.85.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	1.91	1.95	1.98	2.02	2.05	2.09	2.12
C_p (J K^{-1}mol^{-1})	276	281	286	291	296	301	306
Temp. (K)	440						
c_p (J K^{-1}g^{-1})	2.16						
C_p (J K^{-1}mol^{-1})	311						

Name: 2–Naphthol
Formula: $C_{10}H_8O$

CAS–RN: 135–19–3
Group No.: 42–086
Molar Mass: 144.17

TABLE 42.86.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	394.0–478.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 42.86.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
394.0–478.0		1.68962+1	4.52896				V

TABLE 42.86.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450	460
c_p (J K^{-1}g^{-1})	2.02	2.05	2.07	2.10	2.12	2.15	2.18
C_p (J K^{-1}mol^{-1})	291	295	299	302	306	310	314
Temp. (K)	470	480					
c_p (J K^{-1}g^{-1})	2.20	2.23					
C_p (J K^{-1}mol^{-1})	317	321					

Name: 2–Methyl–5–(1–methylethyl)phenol
Formula: $C_{10}H_{14}O$

CAS–RN: 499–75–2
Group No.: 42–087
Molar Mass: 150.22

TABLE 42.87.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
05LOU	N	401.65	2.414	nosp	not specified		C_{avg}	DSIO	*98LOU

05LOU average value in temperature range 297–506 K

Name: 3,7–Dimethyl–6–octen–1–yn–3–ol
Formula: $C_{10}H_{16}O$

CAS–RN: 29171–20–8
Group No.: 42–088
Molar Mass: 152.24

TABLE 42.88.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.4–333.6	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 42.88.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.241	2.23–1	0.48	9.97–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
273.4–333.6		2.70946+1	6.04386				V

TABLE 42.88.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	2.37	2.38	2.40	2.44	2.46	2.47	2.50
C_p ($J\,K^{-1}mol^{-1}$)	361	363	366	371	375	376	381
Temp. (K)	320	330					
c_p ($J\,K^{-1}g^{-1}$)	2.54	2.57					
C_p ($J\,K^{-1}mol^{-1}$)	386	391					

Name: 3,7–Dimethyl–1,6–octadien–3–ol
Formula: $C_{10}H_{18}O$

CAS–RN: 78–70–6
Group No.: 42–089
Molar Mass: 154.25

TABLE 42.89.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
33KOL/UDO	N	293.10	2.415	nosp	not	specified	C_p	BSIT	34KOL/UDO2

33KOL/UDO same datum in 34KOL/UDO2

Name: 1–Decanol
Formula: $C_{10}H_{22}O$

CAS–RN: 112–30–1
Group No.: 42–090
Molar Mass: 158.28

TABLE 42.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67GRA	308.1–338.1	4	1.00	not specified		C_p	BSIO	67GRA
75WOY/KAL	303.1	1	nosp	not specified		C_p	BSIO	70REC
79GRI/YAN	305.8–463.3	9	0.90	not specified		C_p	BDAO	75RAS/GRI
79SVE	301.0–461.0	33S	nosp	99.80	chrom	C_{sat}	BDHT	69PER/COM
80VAS/TRE	323.0–403.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	403.0–503.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE
85COS/PAT8	283.1–313.1	3	nosp	99.	estim	C_p	FSIT	71PIC/LED
88AND/PAT	298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED
88NAZ/BAS	304.0–523.0	9	2.20	99.1	anal	C_p	BDHO	86NAZ/BAS1

TABLE 42.90.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75WOY/KAL	303.1	1	0.50#	0.257	5.83–2	0.13	5.83–2	1
79GRI/YAN	305.8–463.3	9	0.90	1.046	5.34–1	0.94	3.82–1	5
79SVE	301.0–461.0	33	1.50#	0.389	3.31–1	0.58	–2.54–1	–25
80VAS/TRE	403.0–503.0	11	3.00#	0.170	3.06–1	0.51	–2.42–1	–9
85COS/PAT8	283.1–313.1	3	0.50#	0.610	1.41–1	0.31	–1.19–1	–3
88AND/PAT	298.1	1	0.50#	1.305	2.93–1	0.65	2.93–1	1
				Rejected data				
67GRA	(1.70, 3.74,–1.58, –4)		80VAS/TRE	(6.78–1, 1.31,–6.54–1, –8)				
88NAZ/BAS	(1.89, 3.19, 1.41–1, –2)							

TABLE 42.90.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	79	58	0.583	3.73–1	0.66	–1.31–1	–3 0

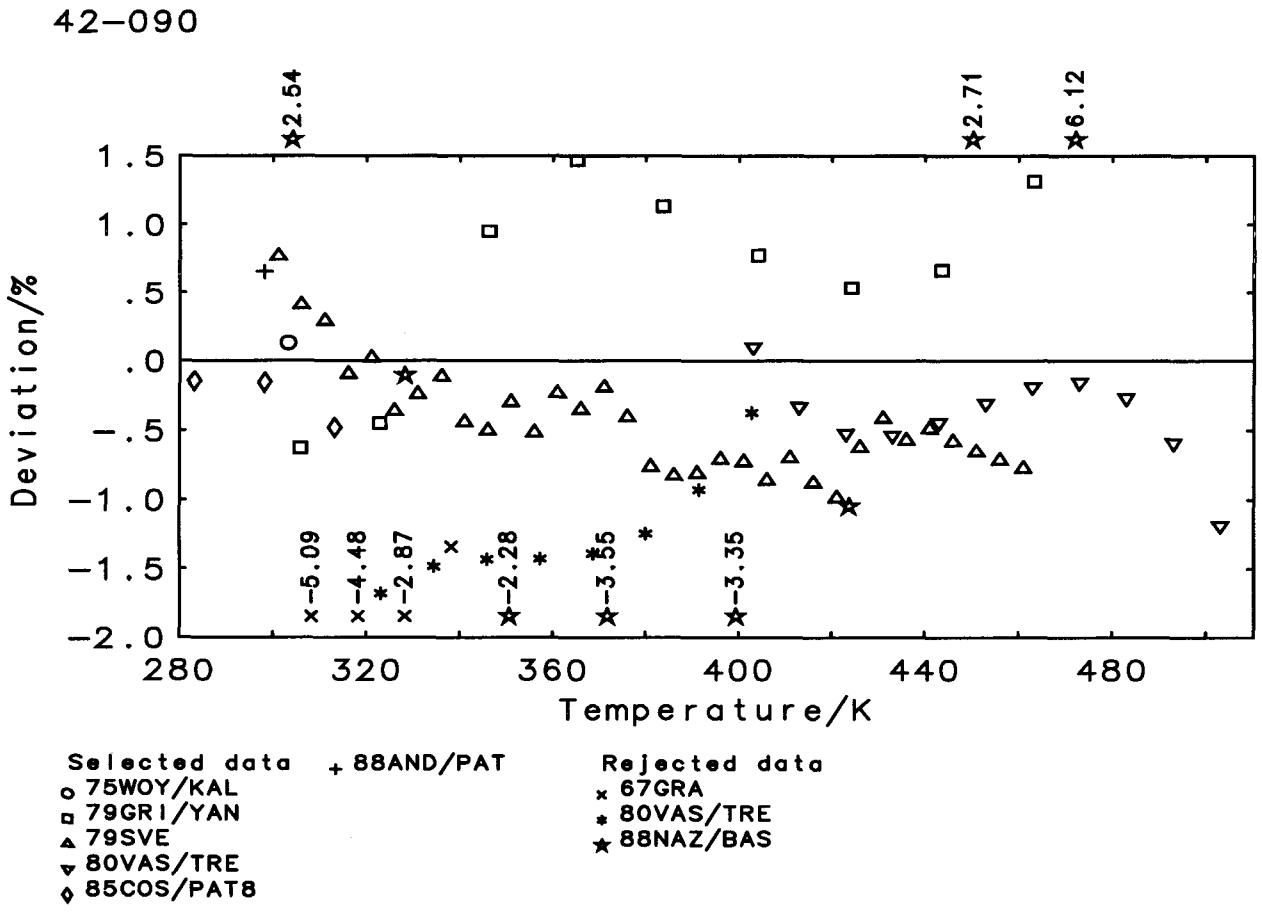
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
283.1–400.0	1.57206+2	–1.32842+2	4.60931+1	–4.76567	IV
400.0–503.0	–5.53844+2	4.00445+2	–8.72287+1	6.34448	V

TABLE 42.90.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	2.206	2.278	2.341	2.356	2.436	2.518	2.601
C ($J K^{-1} mol^{-1}$)	349.2	360.6	370.5	372.9	385.6	398.6	411.7
Temp. (K)	340	350	360	370	380	390	400
c ($J K^{-1} g^{-1}$)	2.683	2.761	2.836	2.905	2.967	3.020	3.064
C ($J K^{-1} mol^{-1}$)	424.6	437.1	448.9	459.9	469.7	478.1	484.9
Temp. (K)	410	420	430	440	450	460	470
c ($J K^{-1} g^{-1}$)	3.10	3.12	3.13	3.14	3.15	3.15	3.16
C ($J K^{-1} mol^{-1}$)	490	494	496	497	498	499	499
Temp. (K)	480	490	500				
c ($J K^{-1} g^{-1}$)	3.16	3.17	3.19				
C ($J K^{-1} mol^{-1}$)	500	502	505				

TABLE 42.90.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	79	58	0.905	4.53–1	0.83	4.10–2	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
283.1–503.0	689.00	2.94700+2	4.25818+1	–8.39157+1	5.09888+2		V



Name: 5–Decanol
Formula: $C_{10}H_{22}O$

CAS–RN: 5205–34–5
Group No.: 42–091
Molar Mass: 158.28

TABLE 42.91.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	2.564	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 3,7–Dimethyl–1–octanol
Formula: $C_{10}H_{22}O$

CAS–RN: 106–21–8
Group No.: 42–092
Molar Mass: 158.28

TABLE 42.92.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	2.320	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 4–Propyl–4–heptanol
Formula: $C_{10}H_{22}O$

CAS–RN: 2198–72–3
Group No.: 42–093
Molar Mass: 158.28

TABLE 42.93.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88CAC/COS	298.15	2.822	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 1–Undecanol
Formula: $C_{11}H_{24}O$

CAS–RN: 112–42–5
Group No.: 42–094
Molar Mass: 172.31

TABLE 42.94.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82VAS/PET	303.0–433.0	eqn	nosp	99.7	anal	C_{sat}	BSAO	80VAS/TRE
82VAS/PET	433.0–523.0	eqn	nosp	99.7	anal	C_{sat}	BSAO	80VAS/TRE
87NAZ/BAD	303.6–499.6	9	nosp	not specified		C_p	BDHO	86NAZ/BAS1
88AND/PAT	298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

TABLE 42.94.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82VAS/PET	303.0–433.0	14	3.00#	0.148	2.39–1	0.44	4.39–2	0
82VAS/PET	433.0–523.0	10	3.00#	0.091	1.79–1	0.27	1.95–2	–1
88AND/PAT	298.1	1	0.50#	0.088	2.14–2	0.04	–2.14–2	–1
				Rejected data				
87NAZ/BAD	(2.92, 4.39, 1.45–3, –3)							

TABLE 42.94.3. Parameters of cubic spline polynomials

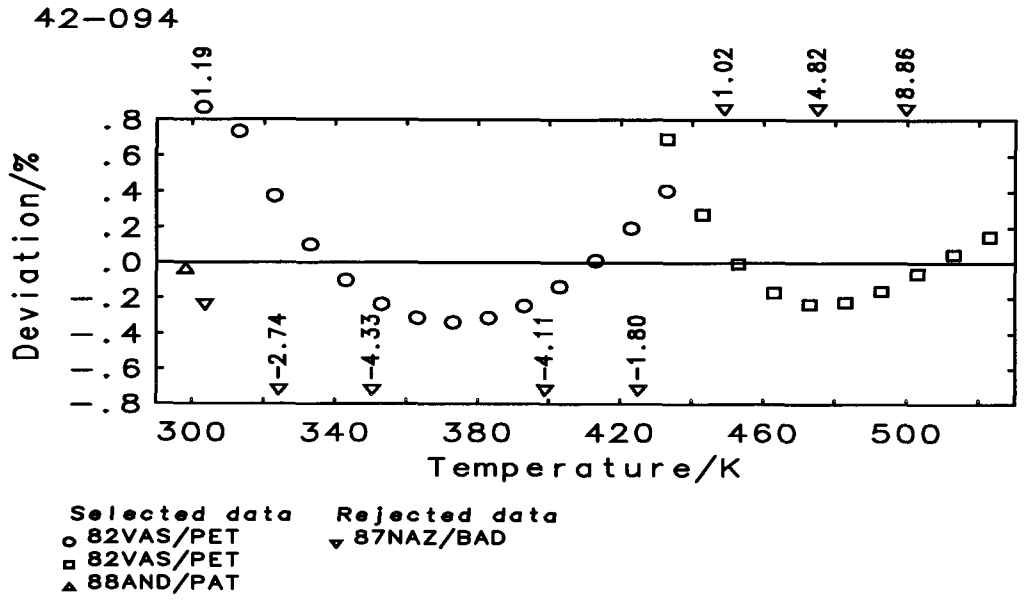
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	34	25	0.141	2.37–1	0.42	3.15–2	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
298.1–420.0		–7.44262+1	6.37119+1	–7.99414	1.66938–1		V
420.0–523.0		–2.32560+2	1.76665+2	–3.48877+1	2.30135		V

TABLE 42.94.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c ($J K^{-1}g^{-1}$)	2.38	2.47	2.56	2.64	2.72	2.79	2.85
C ($J K^{-1}mol^{-1}$)	410	426	441	455	468	481	492
Temp. (K)	370	380	390	400	410	420	430
c ($J K^{-1}g^{-1}$)	2.91	2.96	3.01	3.05	3.08	3.11	3.14
C ($J K^{-1}mol^{-1}$)	502	511	519	525	531	536	540
Temp. (K)	440	450	460	470	480	490	500
c ($J K^{-1}g^{-1}$)	3.15	3.17	3.18	3.19	3.19	3.19	3.20
C ($J K^{-1}mol^{-1}$)	544	546	548	549	550	550	551
Temp. (K)	510	520					
c ($J K^{-1}g^{-1}$)	3.20	3.20					
C ($J K^{-1}mol^{-1}$)	551	551					

TABLE 42.94.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	34	25	0.336	1.95–1	0.34	–4.37–2	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
298.1–523.0	705.00	3.35257+2	4.95960+1	–9.19983+1	5.66565+2		V



Name: 1–Dodecanol
Formula: $C_{12}H_{26}O$

CAS–RN: 112–53–8
Group No.: 42–095
Molar Mass: 186.34

TABLE 42.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79SVE	316.0–486.0	35S	nosp	99.98	chrom	C_{sat}	BDHT	69PER/COM
82VAS/PET	303.0–423.0	eqn	nosp	99.9	anal	C_{sat}	BSAO	80VAS/TRE
82VAS/PET	423.0–533.0	eqn	nosp	99.9	anal	C_{sat}	BSAO	80VAS/TRE
88AND/PAT	298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

TABLE 42.95.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79SVE	316.0–486.0	35	1.50#	0.108	1.04–1	0.16	–1.55–3	–7
88AND/PAT	298.1	1	0.50#	0.028	7.29–3	0.01	7.29–3	1
				Rejected data				
82VAS/PET	(2.59, 4.01, 2.58, 12)		82VAS/PET	(2.61, 3.68, 2.61, 6)				

TABLE 42.95.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	59	36	0.115	1.10–1	0.17	–1.30–3	–6
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
298.1–400.0		1.35666+2	–1.09285+2	3.99551+1	–4.23656		V
400.0–486.0		–5.47885+2	4.03378+2	–8.82106+1	6.44392		V

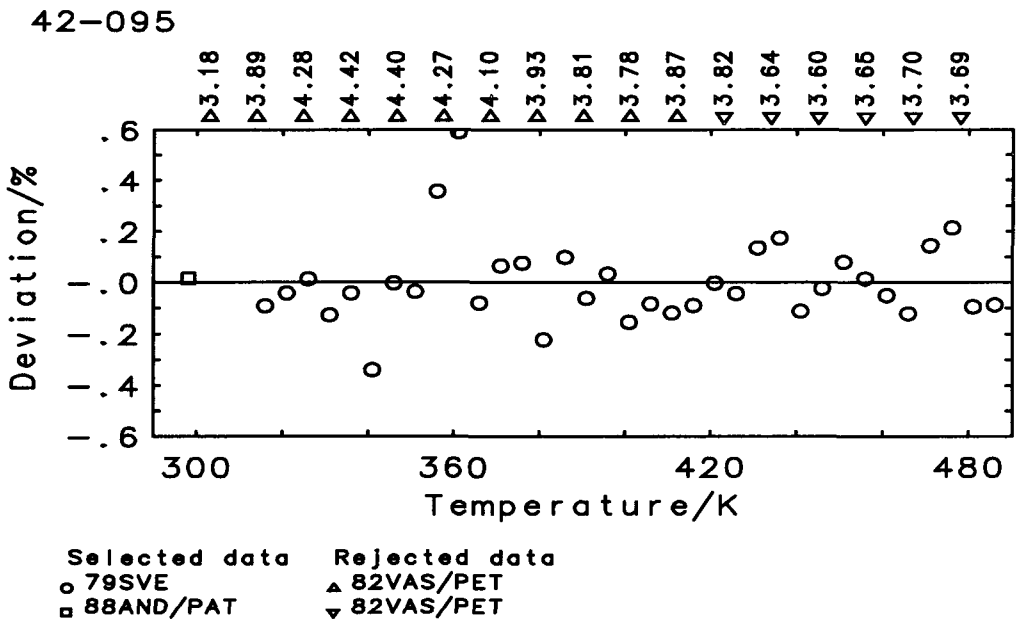
TABLE 42.95.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_{sat} (J K^{-1}g^{-1})	2.37	2.44	2.51	2.58	2.65	2.72	2.78
C_{sat} (J K^{-1}mol^{-1})	441	454	468	481	494	507	519
Temp. (K)	370	380	390	400	410	420	430
c_{sat} (J K^{-1}g^{-1})	2.84	2.89	2.94	2.97	3.00	3.02	3.03
C_{sat} (J K^{-1}mol^{-1})	530	539	548	554	559	563	565
Temp. (K)	440	450	460	470	480	490	
c_{sat} (J K^{-1}g^{-1})	3.04	3.05	3.05	3.05	3.06	3.07	
C_{sat} (J K^{-1}mol^{-1})	567	567	568	569	570	572	

TABLE 42.95.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	59	36	0.446	2.21–1	0.37	–1.36–2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
298.1–486.0	720.00	5.25751+2	8.70909+1	–1.44019+2	7.93465+2	V



Name: 5–Butyl–5–nonanol
Formula: $C_{13}H_{28}O$

CAS–RN: 597–93–3
Group No.: 42–096
Molar Mass: 200.36

TABLE 42.96.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88CAC/COS	298.15	2.738	nosp	not specified		C_p	FSIT	71PIC/LED

Name: 1–Tridecanol
Formula: $C_{13}H_{28}O$

CAS–RN: 112–70–9
Group No.: 42–097
Molar Mass: 200.36

TABLE 42.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74MOS/MOU	305.0–346.0	eqn	nosp	99.97	chrom	C_p	BSAO	74MOS/MOU
80VAS/TRE	323.0–423.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	423.0–553.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE

TABLE 42.97.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74MOS/MOU	305.0–345.8	9	0.50#	0.155	4.88–2	0.08	–1.04–2	0
80VAS/TRE	323.0–423.0	11	2.00	0.255	3.38–1	0.51	1.92–1	8
80VAS/TRE	423.0–553.0	14	2.00	0.191	2.84–1	0.38	–3.88–2	–2

TABLE 42.97.3. Parameters of cubic spline polynomials

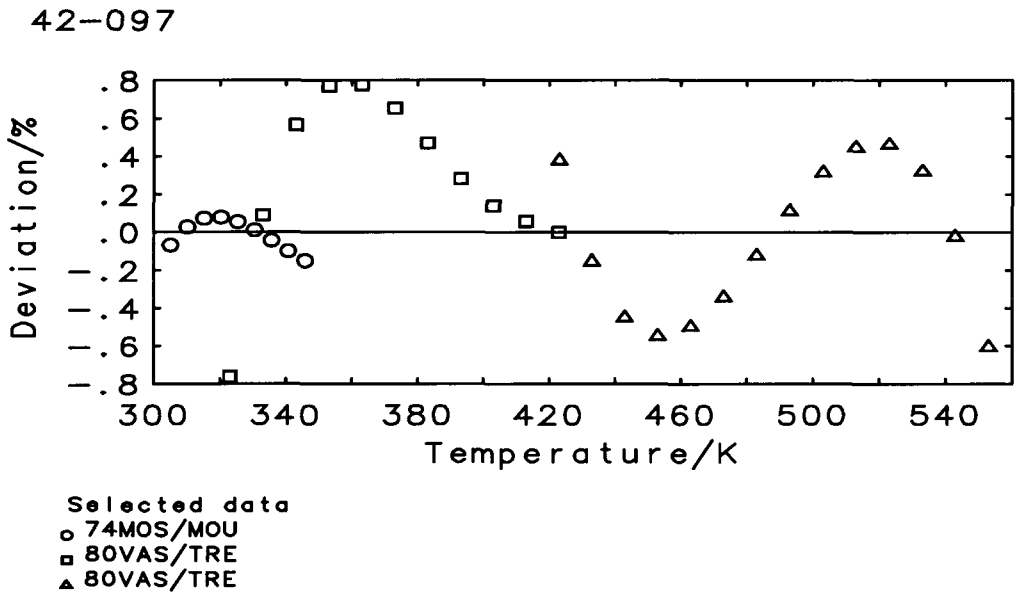
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	34	0.223	2.88–1	0.41	4.35–2	6
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
305.0–400.0		2.61879+2	–2.08976+2	6.67144+1	-6.58424		V
400.0–553.0		–5.09090+2	3.69251+2	–7.78424+1	5.46216		V

TABLE 42.97.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J $K^{-1}g^{-1}$)	2.45	2.51	2.58	2.65	2.71	2.78	2.84
C_{sat} (J $K^{-1}mol^{-1}$)	491	504	517	530	544	557	569
Temp. (K)	380	390	400	410	420	430	440
c_{sat} (J $K^{-1}g^{-1}$)	2.90	2.95	2.99	3.02	3.04	3.06	3.07
C_{sat} (J $K^{-1}mol^{-1}$)	581	591	599	605	610	612	614
Temp. (K)	450	460	470	480	490	500	510
c_{sat} (J $K^{-1}g^{-1}$)	3.07	3.07	3.07	3.07	3.07	3.07	3.07
C_{sat} (J $K^{-1}mol^{-1}$)	615	615	615	614	614	614	615
Temp. (K)	520	530	540	550			
c_{sat} (J $K^{-1}g^{-1}$)	3.08	3.09	3.12	3.15			
C_{sat} (J $K^{-1}mol^{-1}$)	617	620	624	630			

TABLE 42.97.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	34	0.525	6.38–1	0.90	1.85–1	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
305.0–553.0	734.00	3.93375+2	6.12966+1	–9.79414+1	6.31129+2		V



Name: 1-Tetradecanol
Formula: $C_{14}H_{30}O$

CAS-RN: 112-72-1
Group No.: 42-098
Molar Mass: 214.39

TABLE 42.98.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74MOS/MOU	312.0–346.0	eqn	nosp	99.95	chrom	C_p	BSAO	74MOS/MOU
80VAS/TRE	333.0–413.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	413.0–463.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	463.0–573.0	eqn	2.00	99.2	anal	C_{sat}	BSAO	80VAS/TRE

TABLE 42.98.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74MOS/MOU	312.0–346.2	7	0.50#	0.080	2.58–2	0.04	3.14–3	–2
80VAS/TRE	333.0–412.8	8	2.00	0.502	6.96–1	1.00	1.20–1	2
80VAS/TRE	413.0–463.0	6	2.00	0.275	4.30–1	0.55	–1.01–1	–2
80VAS/TRE	463.0–573.0	12	2.00	0.273	4.35–1	0.55	–4.25–2	–1

TABLE 42.98.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	33	33	0.349	5.09–1	0.69	–4.08–3	–3

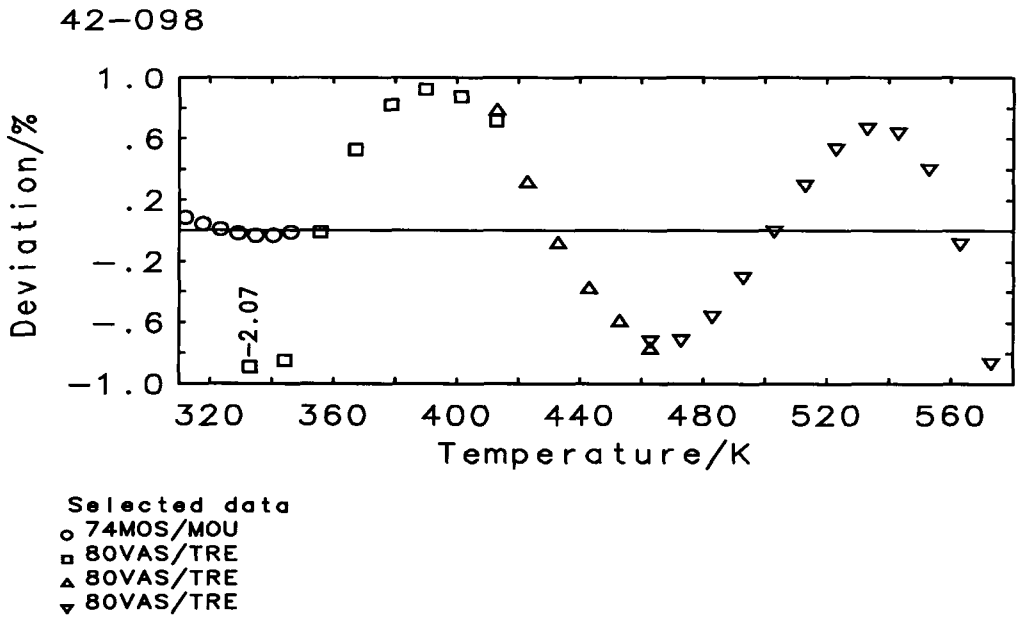
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
312.0–440.0	9.14922+1	–5.90584+1	2.39390+1	–2.54289	V
440.0–573.0	–7.04874+2	4.83918+2	–9.94648+1	6.80588	V

TABLE 42.98.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_{sat} ($J\,K^{-1}g^{-1}$)	2.43	2.49	2.56	2.62	2.68	2.73	2.79
C_{sat} ($J\,K^{-1}mol^{-1}$)	521	535	548	561	574	586	598
Temp. (K)	380	390	400	410	420	430	440
c_{sat} ($J\,K^{-1}g^{-1}$)	2.84	2.89	2.93	2.97	3.00	3.02	3.04
C_{sat} ($J\,K^{-1}mol^{-1}$)	609	619	628	636	643	648	653
Temp. (K)	450	460	470	480	490	500	510
c_{sat} ($J\,K^{-1}g^{-1}$)	3.06	3.06	3.06	3.06	3.06	3.06	3.06
C_{sat} ($J\,K^{-1}mol^{-1}$)	655	656	657	656	656	655	655
Temp. (K)	520	530	540	550	560	570	
c_{sat} ($J\,K^{-1}g^{-1}$)	3.06	3.07	3.09	3.11	3.14	3.19	
C_{sat} ($J\,K^{-1}mol^{-1}$)	656	658	662	667	674	684	

TABLE 42.98.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_{sat}	33	33	0.578	7.72−1	1.02	1.79−1	1 1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
312.0–573.0	747.00	3.66058+2	5.57954+1	−8.59532+1	6.00400+2		V



Name: 4,4'–(1–Methylethylidene)bisphenol
Formula: $C_{15}H_{16}O_2$

CAS–RN: 80–05–7
Group No.: 42–099
Molar Mass: 228.29

TABLE 42.99.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85NOV/TSV	440.0–450.0	2S	5.00	99.7	chrom	C_p	BDHT	74DSM/COM

TABLE 42.99.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
440.0–450.0	5.25586+1	1.20274	VI

TABLE 42.99.4. Recommended values of heat capacities

Temp. (K)	440	450
c_p ($J\,K^{-1}g^{-1}$)	2.11	2.11
C_p ($J\,K^{-1}mol^{-1}$)	481	482

Name: 3,7,11–Trimethyl–1–dodecyn–3–ol
Formula: $C_{15}H_{28}O$

CAS–RN: 1604–35–9
Group No.: 42–100
Molar Mass: 224.39

TABLE 42.100.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.0–343.4	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 42.100.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.052	7.03–2	0.10	–4.77–6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
273.0–343.4	–1.33739+2	1.13484+2	–1.55461+1	V

TABLE 42.100.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	2.20	2.23	2.30	2.39	2.46	2.48	2.54
C_p ($J K^{-1} mol^{-1}$)	493	501	517	537	552	555	571
Temp. (K)	320	330	340				
c_p ($J K^{-1} g^{-1}$)	2.60	2.65	2.68				
C_p ($J K^{-1} mol^{-1}$)	584	594	602				

Name: 1–Pentadecanol
Formula: $C_{15}H_{32}O$

CAS–RN: 629–76–5
Group No.: 42–101
Molar Mass: 228.42

TABLE 42.101.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74MOS/MOU	318.0–346.0	eqn	nosp	99.97	chrom	C_p	BSAO	74MOS/MOU
82VAS/PET	333.0–413.0	eqn	nosp	99.4	anal	C_{sat}	BSAO	80VAS/TRE
82VAS/PET	413.0–513.0	eqn	nosp	99.4	anal	C_{sat}	BSAO	80VAS/TRE
82VAS/PET	513.0–583.0	eqn	nosp	99.4	anal	C_{sat}	BSAO	80VAS/TRE

TABLE 42.101.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74MOS/MOU	318.0–346.0	6	0.50#	0.258	8.98–2	0.13	–3.86–2	–1
82VAS/PET	333.0–413.0	9	3.00#	0.557	1.24	1.67	1.23	9
82VAS/PET	413.0–513.0	11	3.00#	0.282	6.79–1	0.84	–3.52–1	–5
82VAS/PET	513.0–583.0	8	3.00#	0.222	5.65–1	0.67	2.17–1	4

TABLE 42.101.3. Parameters of cubic spline polynomials

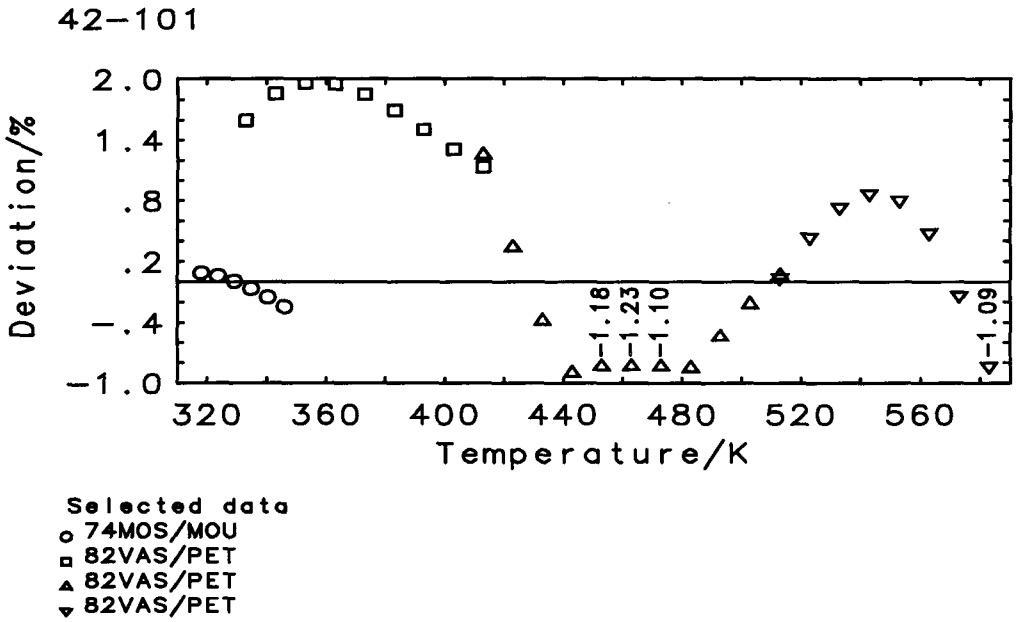
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	34	0.392	8.62–1	1.12	2.56–1	7
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
318.0–450.0		1.62094+2	–1.04154+2	3.33639+1	–3.15939		V
450.0–583.0		–7.93950+2	5.33208+2	–1.08272+2	7.33217		V

TABLE 42.101.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_{sat} ($J K^{-1} g^{-1}$)	2.44	2.48	2.53	2.58	2.63	2.67	2.72
C_{sat} ($J K^{-1} mol^{-1}$)	556	567	578	589	600	611	621
Temp. (K)	390	400	410	420	430	440	450
c_{sat} ($J K^{-1} g^{-1}$)	2.76	2.81	2.85	2.88	2.91	2.93	2.95
C_{sat} ($J K^{-1} mol^{-1}$)	631	641	650	658	665	670	674
Temp. (K)	460	470	480	490	500	510	520
c_{sat} ($J K^{-1} g^{-1}$)	2.96	2.97	2.98	2.98	2.98	2.98	2.99
C_{sat} ($J K^{-1} mol^{-1}$)	677	679	680	680	680	681	682
Temp. (K)	530	540	550	560	570	580	
c_{sat} ($J K^{-1} g^{-1}$)	3.00	3.01	3.03	3.07	3.11	3.17	
C_{sat} ($J K^{-1} mol^{-1}$)	684	688	693	701	710	723	

TABLE 42.101.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	34	34	0.655	1.21	1.49	2.07–1	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
318.0–583.0	759.00	2.17518+2	2.93775+1	–3.45157+1	4.02640+2		V



Name: 1–Hexadecanol
Formula: $C_{16}H_{34}O$

CAS–RN: 36653–82–4
Group No.: 42–102
Molar Mass: 242.45

TABLE 42.102.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74MOS/MOU	323.0–346.0	eqn	nosp	99.96	chrom	C_p	BSAO	74MOS/MOU

TABLE 42.102.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	4.40–6	0.00	–1.53–6	0

Temp. range K	A_1	A_2	Level of uncertainty
323.0–346.2	–1.93932+1	2.76625+1	IV

TABLE 42.102.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	2.466	2.560	2.655
C_p ($J\,K^{-1}mol^{-1}$)	597.8	620.8	643.8

Name: 1–Octadecanol
Formula: $C_{18}H_{38}O$

CAS–RN: 112–92–5
Group No.: 42–103
Molar Mass: 270.50

TABLE 42.103.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80VAS/TRE	353.0–413.0	eqn	2.00	99.8	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	413.0–513.0	eqn	2.00	99.8	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	513.0–623.0	eqn	2.00	99.8	anal	C_{sat}	BSAO	80VAS/TRE

TABLE 42.103.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
80VAS/TRE	353.0–413.0	7	2.00	0.084	1.53–1	0.17	–6.75–2	–4
80VAS/TRE	413.0–513.0	11	2.00	0.080	1.53–1	0.16	5.30–2	3
80VAS/TRE	513.0–623.0	12	2.00	0.044	8.63–2	0.09	–8.25–3	1

TABLE 42.103.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.075	1.43–1	0.15	3.88–4	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
353.0–500.0		-3.80345+2	3.04490+2	-6.51281+1	4 67024		V
500.0–623.0		3.88825+2	-1.57013+2	2.71724+1	-1.48312		V

TABLE 42.103.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c_{sat} (J K^{-1}g^{-1})	2.76	2.80	2.84	2.88	2.90	2.92	2.94
C_{sat} (J K^{-1}mol^{-1})	745	758	769	778	785	791	795
Temp. (K)	430	440	450	460	470	480	490
c_{sat} (J K^{-1}g^{-1})	2.95	2.96	2.97	2.97	2.98	2.99	2.99
C_{sat} (J K^{-1}mol^{-1})	799	801	803	805	806	808	810
Temp. (K)	500	510	520	530	540	550	560
c_{sat} (J K^{-1}g^{-1})	3.00	3.01	3.03	3.05	3.07	3.09	3.11
C_{sat} (J K^{-1}mol^{-1})	812	815	819	824	829	835	842
Temp. (K)	570	580	590	600	610	620	
c_{sat} (J K^{-1}g^{-1})	3.14	3.16	3.19	3.22	3.24	3.27	
C_{sat} (J K^{-1}mol^{-1})	848	855	862	870	877	885	

TABLE 42.103.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.327	6.45–1	0.65	7.07–3	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
353.0–623.0	790.00	9.35743+2	9.43574+1	-2.33365+2	2.03667+3	-1.81534+3	1.77755+3	V

Name: 3,7,11,15–Tetramethyl–1–hexadecyn–3–ol
Formula: $C_{20}H_{38}O$

CAS–RN: 29171–23–1
Group No.: 42–104
Molar Mass: 294.52

TABLE 42.104.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86BER/GUR	N	273.4–333.5	4	2.00	99.	estim	C_p	BDHT	86CDA/COM
87GUR/PET		293.1–343.1	6S	2.00	99.92	chrom	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 42.104.2. Correlated heat capacities

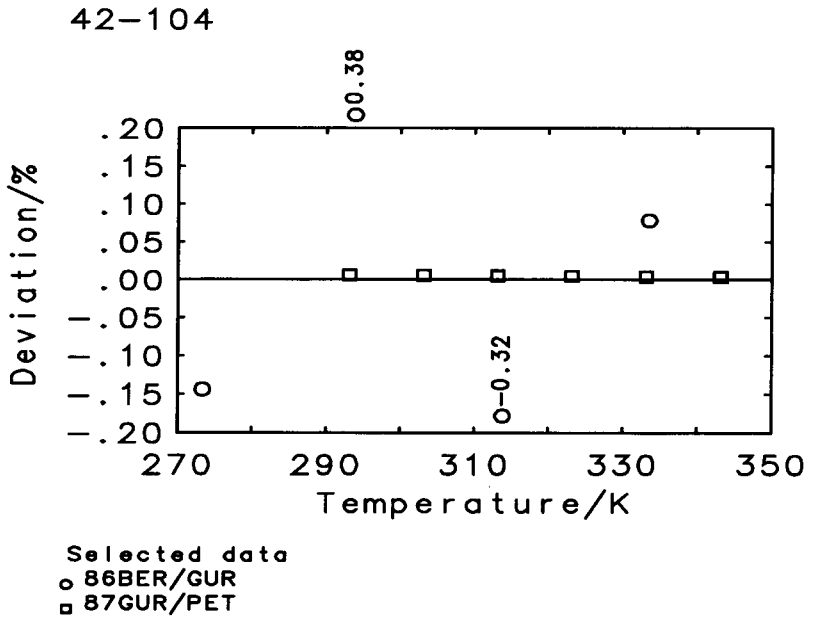
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86BER/GUR	273.4–333.5	4	2.00	0.130	2.25–1	0.26	–2.40–3	0
87GUR/PET	293.1–343.1	6	2.00	0.001	2.46–3	0.00	2.37–3	0

TABLE 42.104.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.092	1.59–1	0.18	4.62–4	0
Temp. range K		A_1	A_2				Level of uncertainty
273.4–343.1		5.63495+1	9.92201				V

TABLE 42.104.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.35	2.36	2.38	2.40	2.43	2.43	2.46
C_p (J K^{-1}mol^{-1})	691	694	700	708	714	716	724
Temp. (K)	320	330	340				
c_p (J K^{-1}g^{-1})	2.49	2.52	2.54				
C_p (J K^{-1}mol^{-1})	733	741	749				



Name: 3,7,11,15-Tetramethyl-1-hexadecen-3-ol
Formula: $C_{20}H_{40}O$

CAS-RN: 505-32-8
Group No.: 42-105
Molar Mass: 296.54

TABLE 42.105.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.0–333.6	4	2.00	99.	estim	C_p	BDHT	86CDA/COM
87GUR/PET		293.1–343.1	6S	2.00	98.74	chrom	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 42.105.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86BER/GUR	273.0–333.6	4	2.00	0.251	4.50–1	0.50	6.78–3	0
87GUR/PET	293.1–343.1	6	2.00	0.007	1.27–2	0.01	–1.69–3	–1

TABLE 42.105.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.190	3.40–1	0.38	1.70–3	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
273.0–343.1	–1.88621+2	1.61103+2	–2.28645+1	V

TABLE 42.105.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.23	2.27	2.33	2.42	2.48	2.49	2.55
C_p (J K^{-1}mol^{-1})	662	672	692	717	735	739	757

Temp. (K)	320	330	340
c_p (J K^{-1}g^{-1})	2.60	2.64	2.66
C_p (J K^{-1}mol^{-1})	771	782	788

43. Carbonyl Compounds

This family contains 64 compounds of which 13 were measured at one temperature only.

The largest number of compounds, 9 ketones as well as benzaldehyde, were measured at NPLT (68AND/COU2, 70AND/COU, 75AMB/CON) and have served as the basis for our recommendations. Comparable reliable data for three ketones originated from DCM (64SIN/OET, 65OET). Six aldehydes were investigated at LSU (83DYA, 83KOR/DYA) having an estimated error of over 1 %. Nine less common ketones which are important for pharmaceutical technology were measured at BTIM over a limited temperature interval and the data showed an uncertainty of 2 % (84BAG/BAE, 86BER/GUR). Data for four higher branched aldehydes were reported by MCSL (87MIL/FEN1, 87MIL/FEN2) and have a claimed error of 1.5 %. Both the old measurements (29KEL3, 32SPA/THO) and more recent values from SUC (56PAR/KEN) have been included in the calculations of recommended values.

For normal C_2 to C_6 aldehydes one to two sharp maxima of the "lambda" type were reported on the C_p=$C_p(T)$ curves determined at CIUG (77KOR/VAS, 88LEB/VAS, 89VAS/LEB, 91VAS/BYK). Such maxima were not found for pentanal, however, the data reported are of low accuracy (83VAS/PET). The complete overview and discussion of these phenomena has been given by Zábranský et al. (93ZAB/BUR). For aldehydes with "lambda" transitions, the correlation had to be carried out over several temperature intervals where narrow ranges of peaks were eliminated; the parameters of the quasipolynomial equation describing the overall temperature range of the experimental data could not be determined for these compounds. Similar transitions may exist for higher molar mass aldehydes, but data of sufficient accuracy are not available. For instance, it is not clear if the kink on the C_p=$C_p(T)$ curve for decanal (83DYA) is due to some transition or just caused by an experimental artifact and no special precaution was taken during the correlation of the data. It was difficult to make a selection for heptanal which was studied at SUC (56PAR/KEL) and at LSU (83DYA); both data sets have a reported error of around 1 %, but differ by 5 to 8 %. The data from SUC have been selected because they seemed to be more reliable.

The most frequently investigated substance was 2-propanone (acetone) for which 17 different sources of data are available containing measurements at more than one temperature. However, the choice for the final correlation was not evident as the results are not consistent and many measurements were performed more than 50 years ago and are of uncertain reliability. The final recommendations are based on the old data from SUC (25PAR/KEL, 29KEL3) for low temperatures, on two data sets near ambient temperatures measured at UCE (62LOW/MOE) and at IKNR (86ALP/PES), and further on, the data from GPI (67RAS/GAN) for temperatures above 333 K. Despite all efforts and a relatively large number of data sources, the recommended values might have an overall error of up to 3 %.

On the other hand, it was possible to make a quite reliable recommendation for 2-butanone (methyl ethyl ketone) where the accurate data were taken from NPLT (68AND/COU2) and from DCM (64SIN/OET) and also supplemented at superambient temperatures with the data from GPI (67RAS/GAN). The recommendations for cyclohexanone based on measurements from UOTO (80NAK/SUG) show an uncertainty of around 0.3 %. Similarly, recommended data for 2-octanone based on experimental values from DCM (65OET) have an estimated error near 0.3 %.

Name: Acetaldehyde
Formula: C_2H_4O

CAS–RN: 75–07–0
Group No.: 43–001
Molar Mass: 44.05

TABLE 43.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47CON/ELV		273.1	1	1.00	99.	anal	C_p	BSIO	49WEI
88LEB/VAS	N	149.8–300.0	16	0.20	99.83	melpt	C_p	BSAO	76LEB/LIT

88LEB/VAS transition at 242.9 K

TABLE 43.1.2a. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88LEB/VAS	149.8–240.0	9	0.20	2.691	6.40–2	0.54	9.82–4	–1

TABLE 43.1.2b. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88LEB/VAS	260.0–300.0	6	0.20	0.216	4.47–3	0.04	4.29–6	0
				Rejected data				
47CON/ELV	(1.44, 12.43, 1.44, 1)							

TABLE 43.1.3a. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	9	4.036	9.59–2	0.81	9.82–4	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
149.8–215.0		–3.45299+1	7.64849+1	–4.75608+1	1.00917+1		II
215.0–240.0		–2.23539+3	3.14745+3	–1.47591+3	2.31542+2		IV

TABLE 43.1.3b. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	6	0.265	5.47–3	0.05	4.29–6	0
C_{sat}	17	6	0.256	5.31–3	0.05	3.66–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
260.0–300.0		3.86986	2.29320				II
260.0–300.0		3.98383	2.24937				II

TABLE 43.1.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.367	1.402	1.439	1.491	1.570	1.685	1.850
C_p (J K^{-1}mol^{-1})	60.24	61.74	63.39	65.69	69.14	74.25	81.52
Temp. (K)	220	230	240				
c_p (J K^{-1}g^{-1})	2.081	2.514	3.407				
C_p (J K^{-1}mol^{-1})	91.68	110.8	150.1				
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.856	1.899	1.913	1.942	1.986	2.021	2.029
C_p (J K^{-1}mol^{-1})	81.75	83.66	84.26	85.56	87.47	89.02	89.38
c_{sat} (J K^{-1}g^{-1})	1.856	1.898	1.912	1.941	1.983	2.018	2.026
C_{sat} (J K^{-1}mol^{-1})	81.75	83.62	84.21	85.49	87.36	88.88	89.23

Name: 1,2–Propadiene–1,3–dione
Formula: C_3O_2

CAS–RN: 504–64–3
Group No.: 43–002
Molar Mass: 68.03

TABLE 43.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65MCD/KIL2	N	167.4–243.1	8	nosp	99.977	melpt	C_p	BSIO	55TAY/JOH

65MCD/KIL2 corrected for Carbon dioxide content

TABLE 43.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.196	7.03–3	0.06	4.89–6	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
167.4–243.1	1.57556+1	–4.10909	1.09008	III

TABLE 43.2.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.457	1.453	1.452	1.454	1.458	1.466	1.475
C_p (J K^{-1}mol^{-1})	99.11	98.87	98.81	98.92	99.22	99.70	100.4

Temp. (K)	240
c_p (J K^{-1}g^{-1})	1.488
C_p (J K^{-1}mol^{-1})	101.2

TABLE 43.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	6	0.323	1.16–2	0.10	1.13–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
188.4–243.1	446.00	2.63142+1	9.27232	2.37482	1.86695+1	III

Name: Propanal
Formula: C_3H_6O

CAS–RN: 123–38–6
Group No.: 43–003
Molar Mass: 58.08

TABLE 43.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	301.7–309.5	4S	nosp	not specified		C_{avg}	DSIO	*81VON
77KOR/VAS	171.3–335.0	12S	nosp	99.4	melpt	C_p	BSAO	77KU/COM
80FUC	298.2	1	0.50	not specified		C_p	BSIO	80FUC

TABLE 43.3.2a. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
77KOR/VAS	171.3–286.0	8	2.00#	1.830	6.97–1	3.66	5.11–2	0

TABLE 43.3.2b. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
77KOR/VAS	286.0–335.0	5	2.00#	0.104	4.10–2	0.21	2.01–4	–1
				Rejected data				
*81VON	(2.18, 13.31, –2.16, –4)		80FUC	(2.67, 16.15, –2.67, –1)				

TABLE 43.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	8	2.315	8.81–1	4.63	5.11–2	0
C_p	17	5	0.164	6.48–2	0.33	2.01–4	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
171.3–286.0	3.08801+1	–1.60594+1	4.15732	V
286.0–335.0	1.71865+2	–9.35267+1	1.41918+1	V

TABLE 43.3.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	2.21	2.20	2.20	2.22	2.24	2.28	2.33
C_p (J K^{-1}mol^{-1})	128	128	128	129	130	132	135
Temp. (K)	250	260	270	273.15	280		
c_p (J K^{-1}g^{-1})	2.39	2.47	2.55	2.58	2.65		
C_p (J K^{-1}mol^{-1})	139	143	148	150	154		
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.86	2.74	2.72	2.62	2.56	2.54	2.57
C_p (J K^{-1}mol^{-1})	166	159	158	152	149	148	149

Name: 2–Propanone
Formula: C_3H_6O

CAS–RN: 67–64–1
Group No.: 43–004
Molar Mass: 58.08

TABLE 43.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		307.5–321.9	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*98LOU	N	321.9	1	nosp	not specified		C_{avg}	DSIO	*98LOU
07WAL		291.6	1	nosp	not specified		C_p	DSIO	07WAL
12SCH1		233.1–308.1	4	nosp	not specified		C_p	BSIO	12SCH1
12SCH3		253.1–323.1	5	nosp	not specified		C_p	BSIO	12SCH1
16BRA		283.1	1	nosp	not specified		C_{avg}	DSTO	16BRA
21TRE		296.7–319.4	7	nosp	not specified		C_p	BSIO	49WEI
25PAR/KEL		193.2–289.4	10	nosp	not specified		C_p	BSIO	25PAR
25WIL/DAN		293.1–313.1	3S	nosp	not specified		C_p	BSAO	24WIL/DAN
28PAR/KEL		193.2–289.4	10	1.00	not specified		C_p	BSIO	25PAR
29KEL3		180.3–297.0	14	1.00	not specified		C_p	BSIO	29KEL1
29MIT/HAR1		204.8–256.3	24	nosp	not specified		C_p	BSIO	29MIT/HAR1
32TRE	N	298.0	1	nosp	not specified		C_p	BSIO	49WEI
39PHI		302.4	1	nosp	not specified		C_p	BSIO	49WEI
47SKU		293.1	1	0.30	not specified		C_p	BSAO	47SKU
55STA/TUP		287.9–323.7	10	1.00	not specified		C_p	BSAO	55STA/TUP
62LOW/MOE		253.2–308.2	7S	0.50	not specified		C_p	BSIO	57HAR/MOE
67RAS/GAN		293.1–333.1	3S	0.50	not specified		C_p	BSAO	67RAS/GAN
71DES/BHA		298.1–318.1	3S	1.00	not specified		C_p	BSIO	56MUR/VAN
79SAL/PEA		298.1–298.1	2	nosp	not specified		C_p	BSIO	80FUC
80FUC		298.2–298.2	2	0.50	99.	chrom	C_p	BSIO	80FUC
85COS/PAT9		283.1–313.1	3	nosp	99.	chrom	C_p	FSIT	71PIC/LED
86ALP/PES	N	258.1–318.1	4	0.20	not specified		C_p	BSAO	83KUK/KOR
89COS/YAO		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
90YAM/OGA	N	298.1	1	nosp	not specified		C_p	FSIO	85OGA
91GRO/ROU		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED

*98LOU average value in temperature range 293–351 K
32TRE same datum in 33TRE/WAT
86ALP/PES same data in 89PET/PES and 90ALP/PES
90YAM/OGA water content less than 0.02 mol.%

TABLE 43.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
25PAR/KEL	193.2–289.4	10	1.00#	0.329	4.83–2	0.33	–2.11–2	–4
29KEL3	180.3–297.0	14	1.00	0.775	1.12–1	0.77	–6.22–2	–4
62LOW/MOE	253.2–308.2	7	0.50	1.617	1.19–1	0.81	–1.17–1	–7
67RAS/GAN	293.1–333.1	3	0.50	1.226	9.52–2	0.61	6.35–2	1
86ALP/PES	258.1–318.1	4	0.20	1.486	4.41–2	0.30	3.72–2	4
				Rejected data				
*81VON	(9.53–1, 5.78, 9.52–1, 4)			*98LOU	(3.03–1, 1.89, 3.03–1, 1)			
07WAL	(3.37–2, 0.22,–3.37–2, –1)			12SCH1	(2.61–1, 1.84,–5.31–2, 0)			
12SCH3	(1.38–1, 0.93, 2.17–2, 3)			16BRA	(3.45–1, 2.36,–3.45–1, –1)			
21TRE	(6.99–2, 0.46,–3.79–2, –2)			25WIL/DAN	(6.18–1, 3.76, 4.47–1, 3)			
28PAR/KEL	(9.61–2, 0.65,–5.91–2, –4)			29MIT/HAR1	(1.64–1, 1.13, 4.48–2, 1)			
32TRE	(2.00–1, 1.33,–2.00–1, –1)			39PHI	(1.86–1, 1.20, 1.86–1, 1)			
47SKU	(2.64–1, 1.71, 2.64–1, 1)			55STA/TUP	(2.14–1, 1.37, 2.08–1, 10)			
71DES/BHA	(4.94–1, 3.09, 4.90–1, 3)			79SAL/PEA	(7.03–2, 0.47, –4.91–2, –1)			
80FUC	(1.48–1, 0.98,–1.45–1, –2)			85COS/PAT9	(3.59–1, 2.44,–3.45–1, –3)			
89COS/YAO	(3.06–1, 2.06,–3.06–1, –1)			90YAM/OGA	(3.36–1, 2.26, –3.36–1, –1)			
91GRO/ROU	(3.30–1, 2.22,–3.30–1, –1)							

TABLE 43.4.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	124	38	1.116	1.01–1	0.69	–4.11–2	–10
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.3–260.0		3.09466+1	–2.21705+1	9.34675	–1.24165		IV
260.0–333.1		–2.36004+1	4.07683+1	–1.48605+1	1.86185		IV

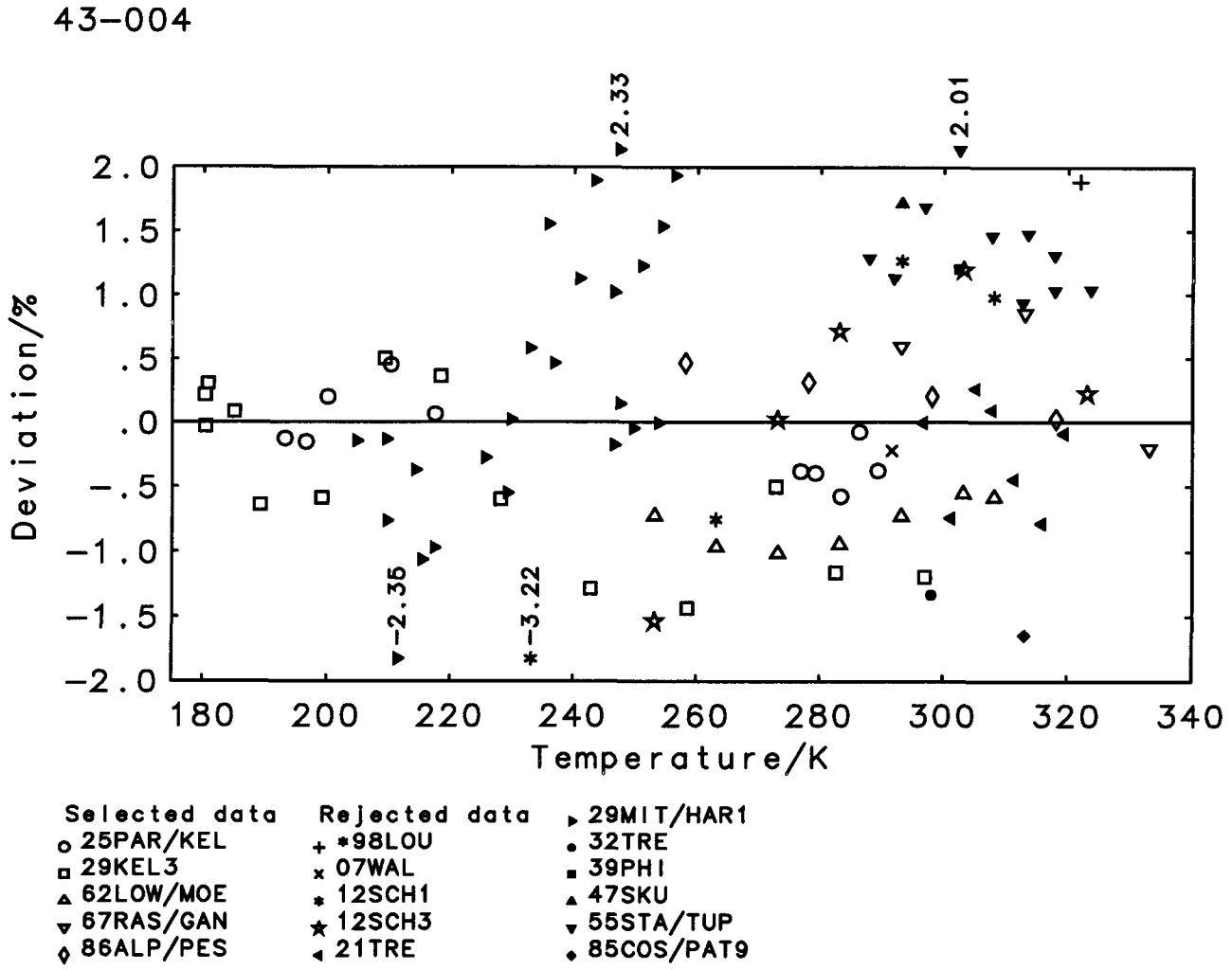
TABLE 43.4.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	2.016	2.011	2.013	2.020	2.031	2.046	2.063
C_p (J K^{-1}mol^{-1})	117.1	116.8	116.9	117.3	118.0	118.8	119.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.081	2.099	2.117	2.123	2.135	2.156	2.175
C_p (J K^{-1}mol^{-1})	120.9	121.9	123.0	123.3	124.0	125.2	126.3
Temp. (K)	300	310	320	330			
c_p (J K^{-1}g^{-1})	2.180	2.210	2.247	2.292			
C_p (J K^{-1}mol^{-1})	126.6	128.4	130.5	133.1			

TABLE 43.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	124	38	1.716	8.20–2	0.56	7.08–3	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
180.3–333.1	508.10	8.02375	1.72437–1	1.25896+1	2.10078+1	–4.13477+1	5.52393+1	IV



Name: 2–Butenal
Formula: C_4H_6O

CAS–RN: 4170–30–3
Group No.: 43–005
Molar Mass: 70.09

TABLE 43.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86BER/GUR	N	273.1–343.5	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 84BAG/BAE and 88BAG/GUR

TABLE 43.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.190	6.86–2	0.38	1.33–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.1–343.5		–1.76272	1.17371+1	–1.71997			V

TABLE 43.5.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.06	2.07	2.09	2.11	2.13	2.13	2.15
C_p (J K^{-1}mol^{-1})	145	145	146	148	149	149	150
Temp. (K)	320	330	340				
c_p (J K^{-1}g^{-1})	2.16	2.16	2.17				
C_p (J K^{-1}mol^{-1})	151	152	152				

Name: Butanal
Formula: C_4H_8O

CAS–RN: 123–72–8
Group No.: 43–006
Molar Mass: 72.11

TABLE 43.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56PAR/KEN	180.0–300.0	13S	1.00	97.7	melpt	C_p	BSIO	25PAR
89VAS/LEB	177.0–330.5	46	0.20	99.26	melpt	C_p	BSAO	76LEB/LIT

TABLE 43.6.2a. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89VAS/LEB	177.0–198.2	9	0.20	1.038	3.63–2	0.21	1.55–4	3
				Rejected data				
56PAR/KEN	(3.29–1, 1.86, 3.10–1, 2)							

TABLE 43.6.2b. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89VAS/LEB	198.2–284.8	27	0.20	5.073	1.85–1	1.01	3.90–3	–3
				Rejected data				
56PAR/KEN	(3.76–1, 2.05, 9.21–2, 5)							

TABLE 43.6.2c. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89VAS/LEB	288.3–330.5	11	0.20	0.728	2.96–2	0.15	6.42–6	0
				Rejected data				
56PAR/KEN	(1.80–1, 0.93,–1.68–1, –2)							

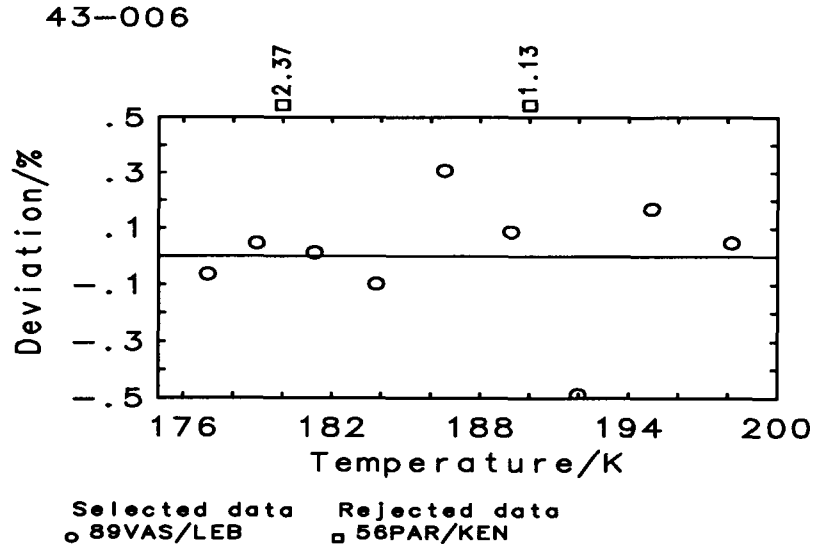
TABLE 43.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	59	9	1.271	4.45–2	0.25	1.55–4	3
C_p	59	27	5.496	2.01–1	1.10	3.90–3	–3
C_p	59	11	0.913	3.71–2	0.18	6.42–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
177.0–198.2	4.58447+1	–3.29807+1	9.50865	0.0	III
198.2–284.8	–5.61809+1	1.05515+2	–5.01737+1	7.91694	IV
288.3–330.5	–5.09016+2	5.16866+2	–1.68781+2	1.84182+1	III

TABLE 43.6.4. Recommended values of heat capacities

Temp. (K)	180	190					
c_p (J K^{-1}g^{-1})	1.993	2.019					
C_p (J K^{-1}mol^{-1})	143.7	145.6					
Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	2.017	2.013	2.008	2.008	2.018	2.044	2.091
C_p (J K^{-1}mol^{-1})	145.4	145.1	144.8	144.8	145.5	147.4	150.8
Temp. (K)	270	273.15	280				
c_p (J K^{-1}g^{-1})	2.165	2.194	2.271				
C_p (J K^{-1}mol^{-1})	156.1	158.2	163.7				
Temp. (K)	290	298.15	300	310	320	330	
c_p (J K^{-1}g^{-1})	2.265	2.285	2.288	2.304	2.325	2.365	
C_p (J K^{-1}mol^{-1})	163.3	164.7	165.0	166.1	167.6	170.5	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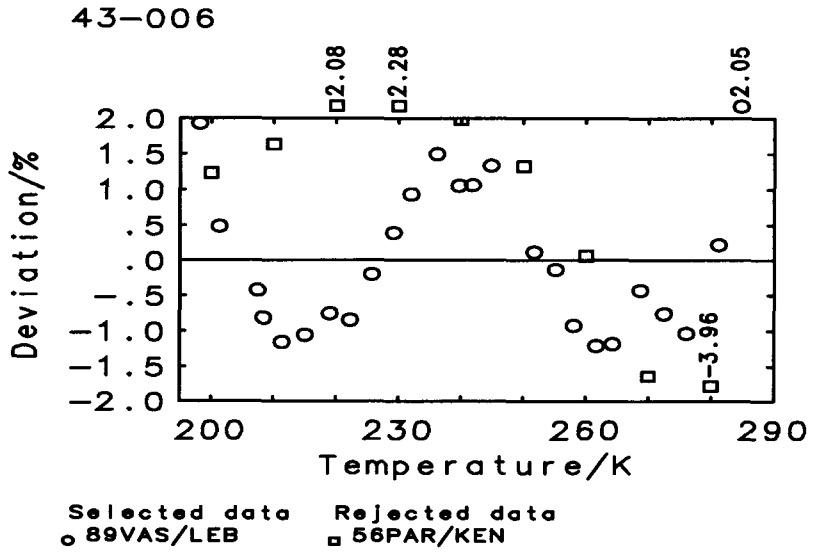
.3
.1
–.1
–.3
–.5
Deviation/%
176
182
188
194
200
Temperature/K
Selected data
o 89VAS/LEB
Rejected data
□ 56PAR/KEN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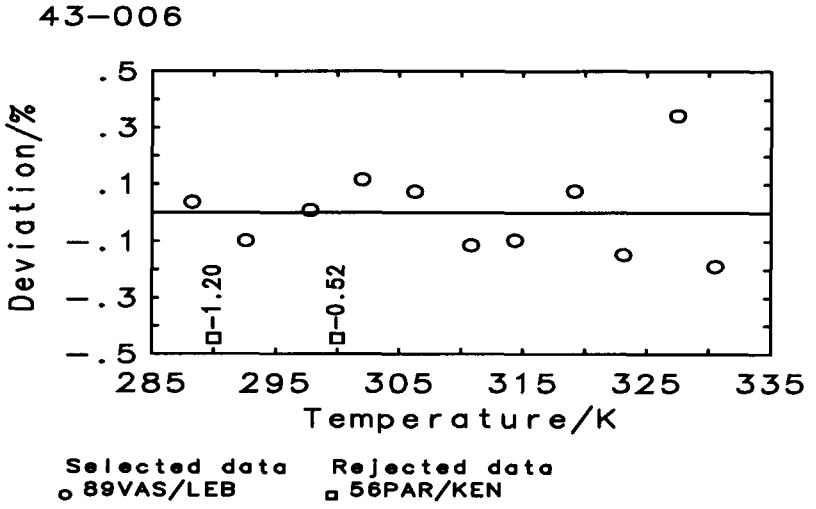
Deviation/%
200
230
260
290
Temperature/K
Selected data
o 89VAS/LEB
Rejected data
□ 56PAR/KEN


43–006
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–1.20
–0.52
Deviation/%
285
295
305
315
325
335
Temperature/K
Selected data
o 89VAS/LEB
Rejected data
□ 56PAR/KEN

Name: 2–Butanone
Formula: C_4H_8O

CAS–RN: 78–93–3
Group No.: 43–007
Molar Mass: 72.11

TABLE 43.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
33KOL/UDO	N	297.0	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified		C_p	not specified	
56PAR/KEN		180.0–300.0	13S	1.00	99.7	melpt	C_p	BSIO	25PAR
64SIN/OET		191.6–336.4	64	0.30	99.78	melpt	C_{sat}	BSAO	58HIL/KRA
67RAS/GAN		293.1–353.1	4S	0.50	not specified		C_p	BSAO	67RAS/GAN
68AND/COU2		190.8–319.8	27	nosp	99.98	melpt	C_{sat}	BSAO	63AND/COU1
75GRO/BEN		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
78ROU/PER1		283.1–313.1	3S	0.30	99.8	chrom	C_p	FSIT	71PIC/LED
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC
84GRO/BEN		298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
85COS/PAT9		283.1–313.1	3	nosp	99.	chrom	C_p	FSIT	71PIC/LED
91KAL/KOH		293.1–313.1	2	1.00	99.89	anal	C_p	FSIT	71PIC/LED

33KOL/UDO same datum in 34KOL/UDO2
38PAN/DUD temperature range of parameters validity estimated by the compilers

TABLE 43.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64SIN/OET	191.6–336.4	64	0.30	0.571	3.18–2	0.17	5.02–3	8
67RAS/GAN	293.1–353.1	4	0.50	0.902	9.05–2	0.45	–6.47–2	–4
68AND/COU2	190.8–319.8	27	0.20#	0.316	1.16–2	0.06	–3.61–3	–10
				Rejected data				
33KOL/UDO	(2.70–1, 1.40, 2.70–1, 1)			38PAN/DUD	(1.40, 7.38,–1.47–1, –1)			
56PAR/KEN	(1.79–1, 0.94, 1.57–1, 11)			75GRO/BEN	(4.79–2, 0.25, 4.79–2, 1)			
78ROU/PER1	(2.34–1, 1.26,–1.31–1, –1)			80FUC	(1.21–1, 0.64,–1.21–1, –1)			
84GRO/BEN	(1.07–1, 0.56,–1.07–1, –1)			85COS/PAT9	(2.34–1, 1.26, –1.31–1, –1)			
91KAL/KOH	(1.59–1, 0.83, 1.23–2, 0)							

TABLE 43.7.3. Parameters of regression polynomial

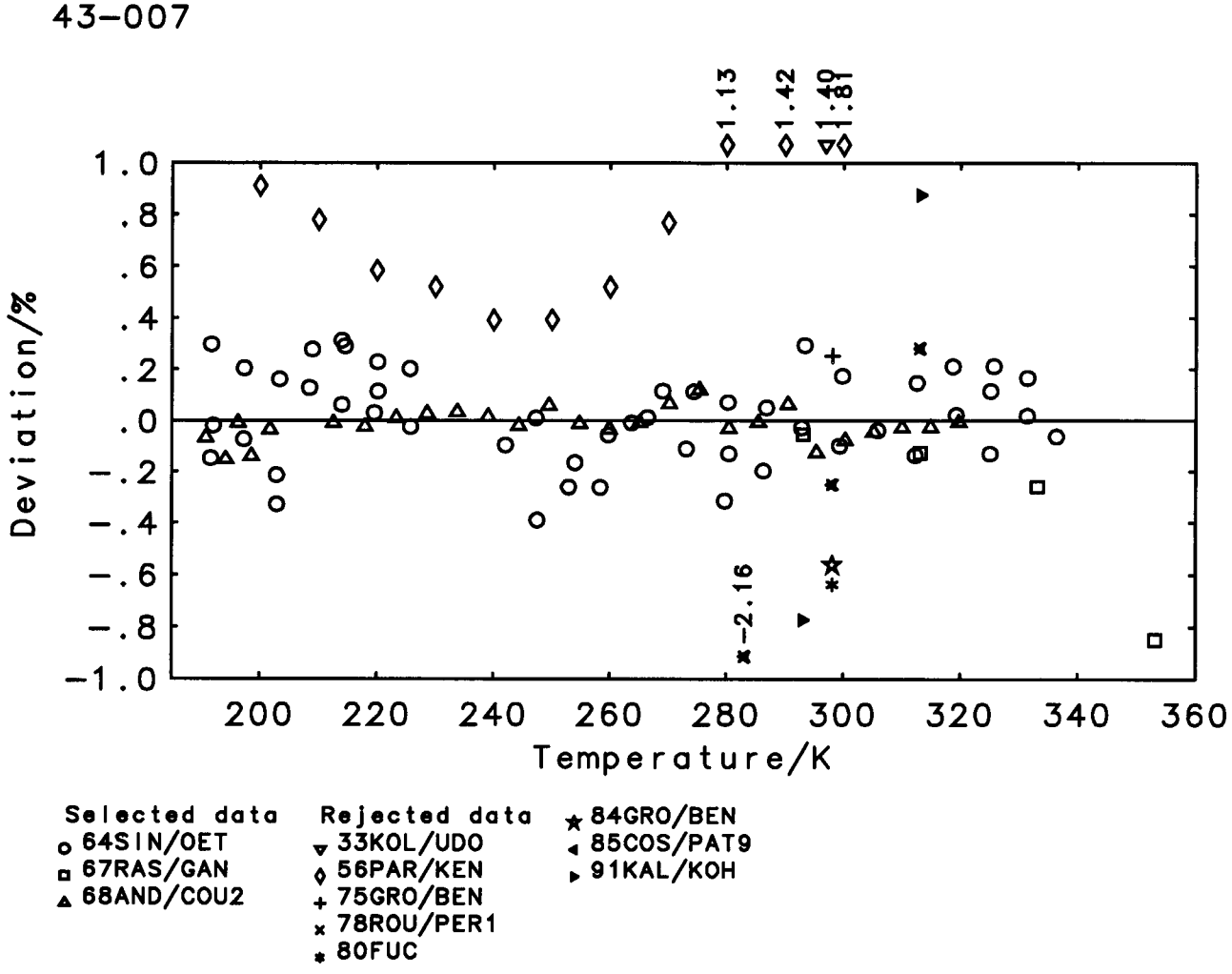
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	126	95	0.543	3.34–2	0.18	–3.68–4	–6
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
190.8–353.1	1.89088+1	–1.32600	3.56943–1	3.66374–2			II

TABLE 43.7.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1}g^{-1}$)	2.067	2.073	2.080	2.088	2.098	2.109	2.121
C_p ($J K^{-1}mol^{-1}$)	149.1	149.5	150.0	150.6	151.3	152.1	153.0
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	2.135	2.151	2.156	2.168	2.186	2.202	2.206
C_p ($J K^{-1}mol^{-1}$)	154.0	155.1	155.5	156.3	157.6	158.8	159.1
Temp. (K)	310	320	330	340	350		
c_p ($J K^{-1}g^{-1}$)	2.228	2.251	2.276	2.302	2.331		
C_p ($J K^{-1}mol^{-1}$)	160.6	162.3	164.1	166.0	168.0		

TABLE 43.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	126	95	0.733	4.26–2	0.23	–3.93–3	–13
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
190.8–353.1	536.78	7.13649–1	2.08950	1.49395+1	6.09350–2		II



Name: Cyclopentanone
Formula: C_5H_8O

CAS–RN: 120–92–3
Group No.: 43–008
Molar Mass: 84.12

TABLE 43.8.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
29KEL4	298.20	1.837	0.50	not specified		C_p	BSIO	29KEL1

Name: 2,4–Pentanedione
Formula: $C_5H_8O_2$

CAS–RN: 123–54–6
Group No.: 43–009
Molar Mass: 100.12

TABLE 43.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69MEL/MER	N	254.8–300.0	8S	nosp	not specified		C_{sat}	BSAO	45SCO/MEY

69MEL/MER predominately enol form

TABLE 43.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.056	3.99–3	0.02	7.15–7	2

Temp. range K	A_1	A_2	Level of uncertainty
254.8–300.0	1.08028+1	4.77614	III

TABLE 43.9.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.928	1.968	1.981	2.008	2.047	2.080	2.087
C_{sat} (J K^{-1}mol^{-1})	193.1	197.0	198.3	201.0	205.0	208.2	209.0

Name: 2,2–Dimethylpropanal
Formula: $C_5H_{10}O$

CAS–RN: 630–19–3
Group No.: 43–010
Molar Mass: 86.13

TABLE 43.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC
83KOR/DYA	N	274.1–350.0	18S	nosp	not specified		C_p	BSAO	77KU/COM

83KOR/DYA error of 0.3–1.0 % reported in 84VAS/PET

TABLE 43.10.2. *Correlated heat capacities*

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
80FUC	298.2	1	0.50	0.543	6.08–2	0.27	6.08–2	1
83KOR/DYA	274.1–350.0	18	0.70#	0.058	9.22–3	0.04	–6.58–3	–12

TABLE 43.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.149	1.81–2	0.08	–3.03–3	–11
Temp. range K		A_1	A_2	A_3			Level of uncertainty
274.1–350.0		1.87883+1	–7.69867–1	6.56880–1			IV

TABLE 43.10.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.103	2.131	2.156	2.161	2.193	2.225	2.259
C_p (J K^{-1}mol^{-1})	181.1	183.6	185.7	186.2	188.9	191.7	194.6
Temp. (K)	340	350					
c_p (J K^{-1}g^{-1})	2.294	2.330					
C_p (J K^{-1}mol^{-1})	197.6	200.7					

TABLE 43.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.148	1.71–2	0.08	–5.99–5	–9
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
274.1–350.0	525.00	–3.49619	5.94823–1	1.51012+1	5.13739		IV

Name: 3–Methyl–2–butanone
Formula: $C_5H_{10}O$

CAS–RN: 563–80–4
Group No.: 43–011
Molar Mass: 86.13

TABLE 43.11.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*98LOU	N	329.0	1	nosp	not specified		C_{avg}	DSIO	*98LOU
68AND/COU2		184.4–323.9	37	nosp	99.6	melpt	C_p	BSAO	63AND/COU1
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC

*98LOU average value in temperature range 293–365 K

TABLE 43.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68AND/COU2	184.4–323.9	37	0.20#	0.472	2.06–2	0.09	3.80–5	5
				Rejected data				
80FUC	(6.53–2, 0.30, 6.53–2, 1)							

TABLE 43.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	37	0.500	2.18–2	0.10	3.80–5	5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
184.4–323.9		2.56413+1	–7.66031	2.84214	–2.41952–1		II

TABLE 43.11.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.897	1.900	1.907	1.916	1.928	1.942	1.958
C_p (J K^{-1}mol^{-1})	163.4	163.7	164.2	165.0	166.0	167.2	168.6
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.976	1.997	2.019	2.026	2.043	2.068	2.090
C_p (J K^{-1}mol^{-1})	170.2	172.0	173.9	174.5	176.0	178.2	180.0
Temp. (K)	300	310	320				
c_p (J K^{-1}g^{-1})	2.095	2.124	2.153				
C_p (J K^{-1}mol^{-1})	180.5	182.9	185.4				

TABLE 43.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	39	37	0.983	4.14–2	0.20	1.42–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
184.4–323.9	553.40	7.57727	6.55080	1.21004+1	2.19115		II

Name: Pentanal
Formula: $C_5H_{10}O$

CAS–RN: 110–62–3
Group No.: 43–012
Molar Mass: 86.13

TABLE 43.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		312.7–340.1	4S	nosp	not specified		C_{avg}	DSIO	*81VON
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC
83KOR/DYA	N	191.6–340.0	17S	nosp	not specified		C_p	BSAO	77KU/COM

83KOR/DYA error above 1.0 % reported in 84VAS/PET

TABLE 43.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83KOR/DYA	191.6–340.0	17	2.00#	0.094	3.98–2	0.19	1.50–4	–1
				Rejected data				
*81VON	(1.70, 7.27, 1.67, 3)			80FUC	(1.78, 7.84, 1.78, 1)			

TABLE 43.12.3. Parameters of regression polynomial

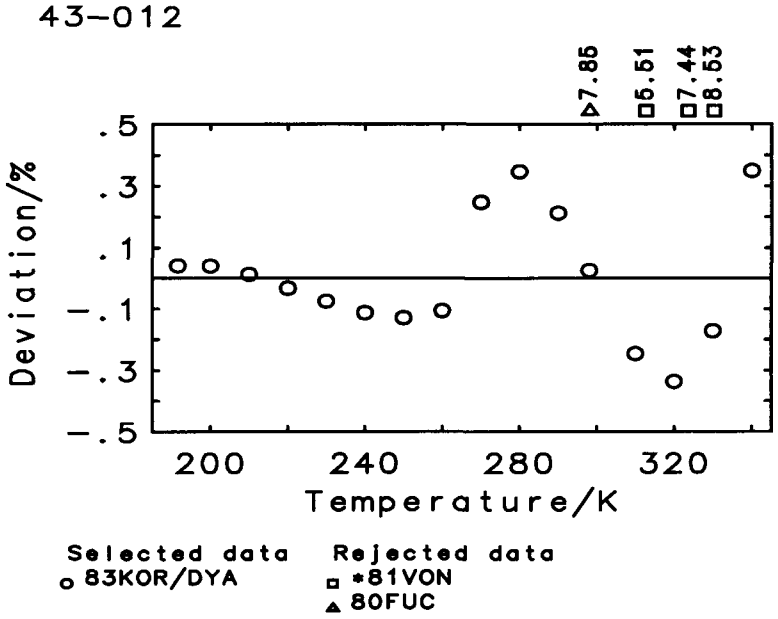
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	17	0.108	4.55–2	0.22	1.50–4	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
191.6–340.0	3.77722+1	–1.95524+1	6.70347	–6.82812–1			V

TABLE 43.12.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.94	1.93	1.93	1.92	1.93	1.93	1.94
C_p (J K^{-1}mol^{-1})	167	166	166	166	166	166	167
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.95	1.97	1.98	1.99	2.01	2.02	2.03
C_p (J K^{-1}mol^{-1})	168	170	170	171	173	174	175
Temp. (K)	310	320	330	340			
c_p (J K^{-1}g^{-1})	2.05	2.07	2.10	2.12			
C_p (J K^{-1}mol^{-1})	177	179	181	182			

TABLE 43.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	14	0.132	5.39–2	0.26	2.22–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
220.0–340.0	554.40	4.56726	4.23995	1.46307+1	1.22996		V



Name: 2–Pentanone
Formula: $C_5H_{10}O$

CAS–RN: 107–87–9
Group No.: 43–013
Molar Mass: 86.13

TABLE 43.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
65OET	202.0–334.0	42	0.30	99.81	melpt	C_{sat}	BSAO	58HIL/KRA
68AND/COU2	200.9–364.1	40	nosp	99.97	melpt	C_{sat}	BSAO	63AND/COU1
70HAR/HEA	298.1	1	nosp	not specified		C_p	not specified	
75GRO/BEN	298.1	1	0.30	not specified		C_p	FSIT	71PIC/LED
79SAL/PEA	298.1	1	nosp	not specified		C_p	BSIO	80FUC
80FUC	298.2	1	0.50	not specified		C_p	BSIO	80FUC

TABLE 43.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65OET	202.0–334.0	42	0.30	0.616	3.99–2	0.18	1.65–3	–2
68AND/COU2	200.9–364.1	40	0.20#	0.464	2.00–2	0.09	–6.63–4	5
				Rejected data				
70HAR/HEA	(7.76–3, 0.03, 7.76–3, 1)			75GRO/BEN	(1.01–1, 0.45, 1.01–1, 1)			
79SAL/PEA	(1.31–1, 0.59, 1.31–1, 1)			80FUC	(1.48–1, 0.66, 1.48–1, 1)			

TABLE 43.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	86	82	0.561	3.26–2	0.15	5.19–4	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.9–364.1		2.96241+1	–1.01103+1	3.44543	–2.99818–1		II

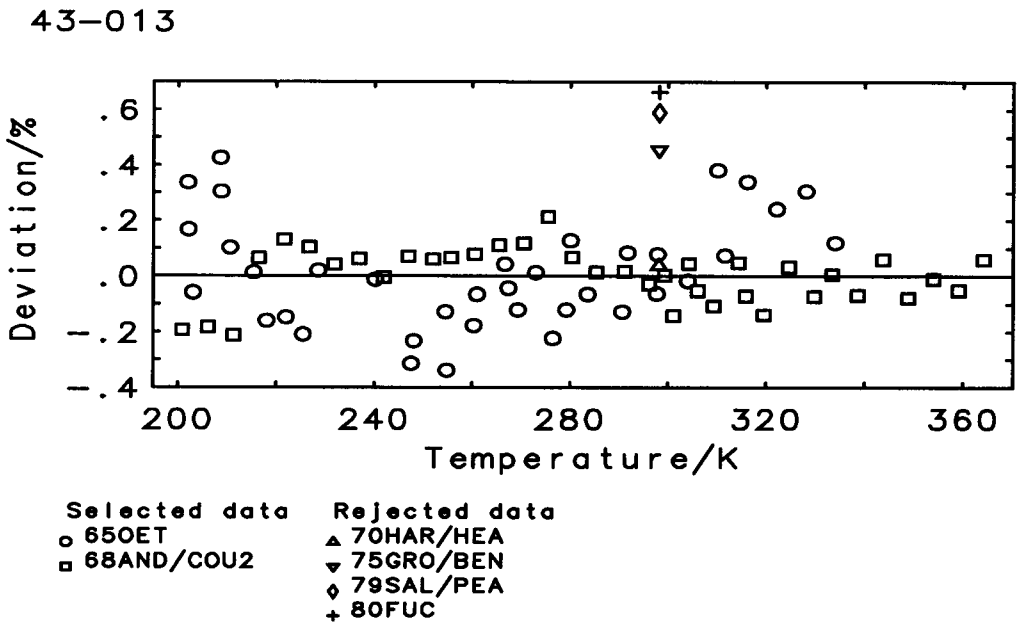
TABLE 43.13.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} ($J K^{-1} g^{-1}$)	2.007	2.009	2.014	2.022	2.033	2.046	2.062
C_{sat} ($J K^{-1} mol^{-1}$)	172.8	173.0	173.5	174.2	175.1	176.2	177.6
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} ($J K^{-1} g^{-1}$)	2.079	2.085	2.099	2.121	2.139	2.144	2.168
C_{sat} ($J K^{-1} mol^{-1}$)	179.1	179.6	180.8	182.7	184.3	184.6	186.8
Temp. (K)	320	330	340	350	360		
c_{sat} ($J K^{-1} g^{-1}$)	2.194	2.221	2.249	2.277	2.306		
C_{sat} ($J K^{-1} mol^{-1}$)	189.0	191.3	193.7	196.1	198.6		

TABLE 43.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	86	82	0.603	3.35–2	0.15	–1.85–4	–6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
200.9–364.1	561.10	2.59960+2	2.23626+1	–5.24961	2.77854+2	–4.70268+1	2.82312+2	II



Name: 3–Pentanone
Formula: $C_5H_{10}O$

CAS–RN: 96–22–0
Group No.: 43–014
Molar Mass: 86.13

TABLE 43.14.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*98LOU	N	332.4	1	nosp	not specified	C_{avg}	DSIO	*98LOU
68AND/COU2		238.4–319.1	24	nosp	99.85 melpt	C_{sat}	BSAO	63AND/COU1
79SAL/PEA		298.1–298.1	2	nosp	not specified	C_p	BSIO	80FUC
80FUC		298.2–298.2	2	0.50	not specified	C_p	BSIO	80FUC
84GRO/BEN		298.1	1	nosp	not specified	C_p	FSIT	71PIC/LED
86BER/GUR	N	274.2–334.6	12	2.00	99. estim	C_p	BDHT	86CDA/COM

*98LOU average value in temperature range 293–372 K
86BER/GUR same data in 84BAG/BAE and some data in 88BAG/GUR

TABLE 43.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
68AND/COU2	238.4–319.1	24	0.20#	0.230	1.04–2	0.05	7.47–6	–1
				Rejected data				
79SAL/PEA	(1.43–1, 0.63,–1.41–1, –2)			80FUC	(1.33–1, 0.58,–1.29–1, –2)			
84GRO/BEN	(7.43–2, 0.32,–7.43–2, –1)			86BER/GUR	(6.19–1, 2.64, 6.10–1, 11)			

TABLE 43.14.3. Parameters of regression polynomial

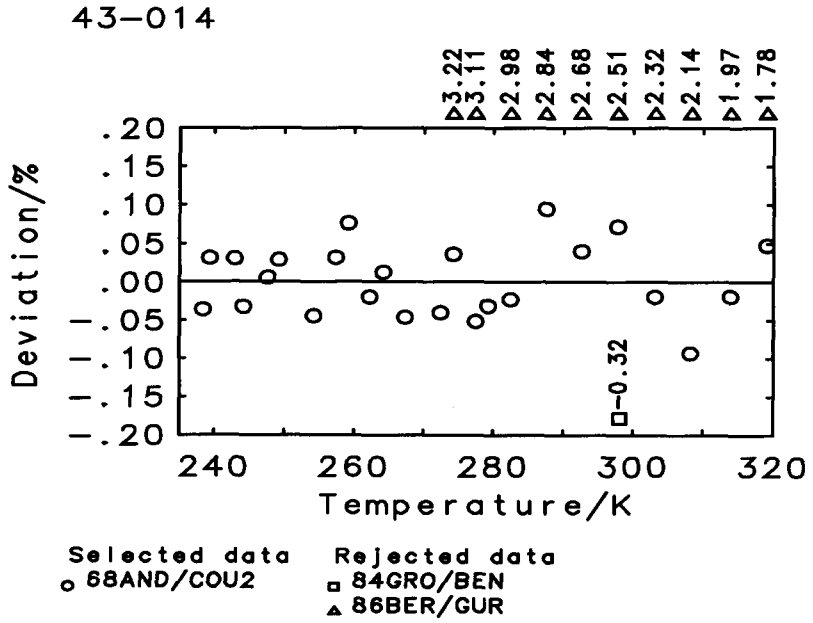
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	42	24	0.252	1.14–2	0.05	7.47–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
238.4–319.1		3.54222+1	–1.54870+1	5.52562	–5.81234–1		II

TABLE 43.14.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	2.128	2.139	2.152	2.167	2.172	2.184	2.201
C_{sat} (J K^{-1}mol^{-1})	183.3	184.2	185.4	186.6	187.1	188.1	189.6
Temp. (K)	298.15	300	310	320			
c_{sat} (J K^{-1}g^{-1})	2.217	2.220	2.239	2.259			
C_{sat} (J K^{-1}mol^{-1})	190.9	191.2	192.9	194.6			

TABLE 43.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	42	24	0.329	1.49–2	0.07	1.73–5	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
238.4–319.1	560.90	1.42821	3.05657	1.74182+1	1.66837–1		II



Name: 2,5–Cyclohexadiene–1,4–dione
Formula: $C_6H_4O_2$

CAS–RN: 106–51–4
Group No.: 43–015
Molar Mass: 108.10

TABLE 43.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	387.0–433.0	*eqn*	*nosp*	*not specified*		C_p	DSIO	26AND/LYN

26AND/LYN probably 1,4 isomer (according to n.m.t.); calculated from temperature dependence of enthalpy by the authors

TABLE 43.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	9.54–7	0.00	–3.82–7	0
Temp. range K		A_1	A_2				Level of uncertainty
387.0–432.9		5.51667	4.42831				V

TABLE 43.15.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430
c_p (J K^{-1}g^{-1})	1.75	1.79	1.82	1.85	1.89
C_p (J K^{-1}mol^{-1})	189	193	197	201	204

Name: 1,4–Cyclohexanedione
Formula: $C_6H_8O_2$

CAS–RN: 637–88–7
Group No.: 43–016
Molar Mass: 112.13

TABLE 43.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DEW/DEK	353.2–358.0	6	nosp	not specified		C_p	BSAO	79SCH/OFF

TABLE 43.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.108	1.16–2	0.04	6.68–6	0
Temp. range K		A_1	A_2				Level of uncertainty
353.2–358.0		2.18273+1	1.40009				III

TABLE 43.16.4. Recommended values of heat capacities

Temp. (K)	352	354	356	358
c_p (J K^{-1}g^{-1})	1.984	1.986	1.988	1.990
C_p (J K^{-1}mol^{-1})	222.5	222.7	222.9	223.2

Name: Cyclohexanone
Formula: $C_6H_{10}O$

CAS-RN: 108-94-1
Group No.: 43-017
Molar Mass: 98.14

TABLE 43.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.6	1	nosp	not specified		C_p	DSIO	22HER/SCH
39PHI	303.9	1	nosp	not specified		C_p	BSIO	49WEI
71VAN	250.0–280.0	7S	nosp	99.95	melpt	C_{sat}	BSAO	72VAN
80FUC	298.2–298.2	2	0.50	not specified		C_p	BSIO	80FUC
80NAK/SUG	244.8–301.4	25	0.30	99.92	melpt	C_{sat}	BSAO	65SUG/SEK

TABLE 43.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
80NAK/SUG	244.8–301.4	25	0.30	0.739	4.29–2	0.22	1.90–4	–6
				Rejected data				
24HER/BLO	(5.23–1, 2.45, 5.23–1, 1)			71VAN	(1.90–1, 0.95, 1.89–1, 7)			
80FUC	(3.70–1, 1.71, 3.66–1, 2)							

TABLE 43.17.3. Parameters of regression polynomial

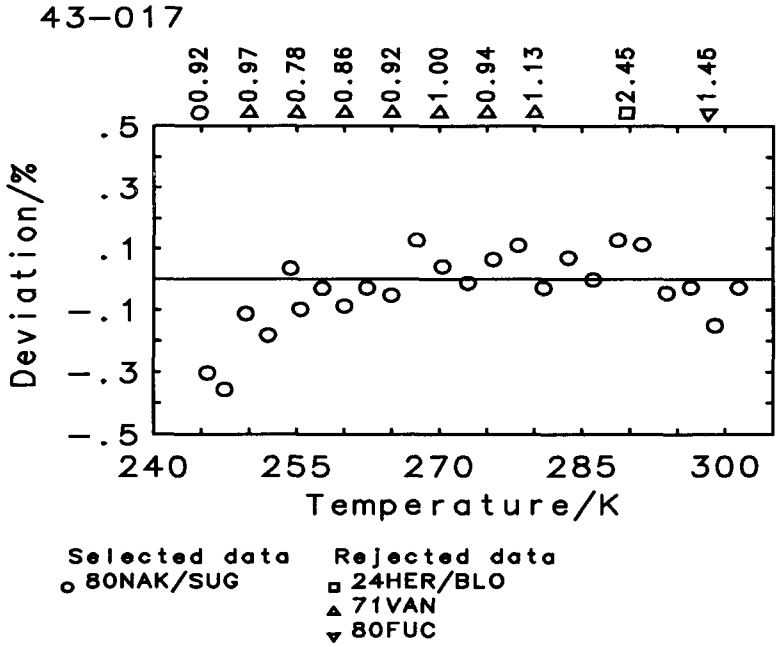
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	36	25	0.787	4.57–2	0.24	1.90–4	–6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
244.8–301.4		1.77097+1	–2.29796	1.16907			II

TABLE 43.17.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J K^{-1} g^{-1}$)	1.633	1.664	1.697	1.707	1.732	1.769	1.800
C_{sat} ($J K^{-1} mol^{-1}$)	160.2	163.3	166.5	167.6	170.0	173.6	176.7
Temp. (K)	300						
c_{sat} ($J K^{-1} g^{-1}$)	1.808						
C_{sat} ($J K^{-1} mol^{-1}$)	177.4						

TABLE 43.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	36	25	0.795	4.62–2	0.24	1.91–4	–6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
244.8–301.4	653.00	2.02306	1.01390+1	3.78024	1.00917–1		II



Name: 4–Methyl–3–penten–2–one
Formula: $C_6H_{10}O$

CAS–RN: 141–79–7
Group No.: 43–018
Molar Mass: 98.14

TABLE 43.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		317.2–354.7	6S	nosp	not specified		C_{avg}	DSIO	*81VON
*98LOU	N	344.1	1	nosp	not specified		C_{avg}	DSIO	*98LOU

*98LOU average value in temperature range 294–394 K

TABLE 43.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
*81VON	317.2–354.7	6	2.00#	0.065	3.31–2	0.13	–2.95–2	–6
*98LOU	344.1	1	3.00#	0.534	4.12–1	1.60	4.12–1	1

TABLE 43.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	7	7	0.249	1.88–1	0.73	3.36–2	–5

Temp. range K	A_1	A_2	Level of uncertainty
317.2–354.7	8.74566	4.81999	V

TABLE 43.18.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	2.05	2.09	2.13	2.17
C ($J\,K^{-1}mol^{-1}$)	201	205	209	213

Name: 3,3–Dimethyl–2–butanone
Formula: $C_6H_{12}O$

CAS–RN: 75–97–8
Group No.: 43–019
Molar Mass: 100.16

TABLE 43.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70AND/COU	226.4–362.8	37	nosp	99.97	melpt	C_{sat}	BSAO	63AND/COU1
80FUC	298.2	1	0.50	not specified		C_p	BSIO	80FUC

TABLE 43.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70AND/COU	226.4–362.8	37	0.20#	0.634	3.28–2	0.13	8.67–5	3
				Rejected data				
80FUC	(3.77–1, 1.49, 3.77–1, 1)							

TABLE 43.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	38	37	0.672	3.48–2	0.13	8.67–5	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
226.4–362.8		3.13399+1	–1.21808+1	4.88727	–5.12708–1		II

TABLE 43.19.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} ($J\,K^{-1}g^{-1}$)	1.904	1.923	1.944	1.967	1.991	1.999	2.017
C_{sat} ($J\,K^{-1}mol^{-1}$)	190.7	192.6	194.7	197.0	199.5	200.2	202.0
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} ($J\,K^{-1}g^{-1}$)	2.043	2.065	2.070	2.098	2.126	2.153	2.181
C_{sat} ($J\,K^{-1}mol^{-1}$)	204.6	206.9	207.4	210.1	212.9	215.7	218.4
Temp. (K)	350	360					
c_{sat} ($J\,K^{-1}g^{-1}$)	2.208	2.234					
C_{sat} ($J\,K^{-1}mol^{-1}$)	221.1	223.7					

TABLE 43.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	38	37	0.952	4.79–2	0.19	1.69–4	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
226.4–362.8	563.80	–3.42151	3.35572–1	1.69854+1	8.72150		II

Name: Hexanal
Formula: $C_6H_{12}O$

CAS–RN: 66–25–1
Group No.: 43–020
Molar Mass: 100.16

TABLE 43.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91VAS/BYK	214.9–330.0	13S	0.20	99.24	melpt	C_p	BSAO	76LEB/LIT

TABLE 43.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
214.9–220.0		3.45363+1	–5.22922				III

TABLE 43.20.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	8	2.292	1.13–1	0.46	3.83–4	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
260.0–298.1		1.24646+3	–1.33049+3	4.80320+2	–5.75013+1		III
298.1–330.0		–2.49867+3	2.43789+3	–7.83601+2	8.38056+1		III

TABLE 43.20.4. Recommended values of heat capacities

Temp. (K)	215	220	225	230			
c_p (J K^{-1}g^{-1})	1.934	1.912	1.890	1.869			
C_p (J K^{-1}mol^{-1})	193.7	191.5	189.3	187.2			
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.952	1.982	1.998	2.036	2.086	2.104	2.103
C_p (J K^{-1}mol^{-1})	195.5	198.5	200.1	204.0	209.0	210.7	210.7
Temp. (K)	310	320	330				
c_p (J K^{-1}g^{-1})	2.078	2.046	2.048				
C_p (J K^{-1}mol^{-1})	208.1	204.9	205.1				

Name: 2–Hexanone
Formula: $C_6H_{12}O$

CAS–RN: 591–78–6
Group No.: 43–021
Molar Mass: 100.16

TABLE 43.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*98LOU	N	347.0	1	nosp	not specified	C_{avg}	DSIO	*98LOU
70AND/COU		220.9–382.6	42	nosp	99.8 melpt	C_{sat}	BSAO	63AND/COU1
80FUC		298.2	1	0.50	not specified	C_p	BSIO	80FUC

*98LOU average value in temperature range 294–400 K

TABLE 43.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70AND/COU	220.9–382.6	42	0.20#	0.527	2.80–2	0.11	5.91–5	–1
				Rejected data				
*98LOU	(7.62–1, 2.73, 7.62–1, 1)			80FUC	(1.50–1, 0.58, 1.50–1, 1)			

TABLE 43.21.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	44	42	0.561	2.98–2	0.11	5.91–5	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
220.9–300.0		4.69483+1	–2.52814+1	8.89981	–9.43358–1		II
300.0–382.6		1.21815+1	9.48547	–2.68914	3.44303–1		II

TABLE 43.21.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} ($J K^{-1}g^{-1}$)	2.022	2.026	2.033	2.044	2.059	2.075	2.081
C_{sat} ($J K^{-1}mol^{-1}$)	202.5	202.9	203.7	204.8	206.2	207.9	208.4
Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} ($J K^{-1}g^{-1}$)	2.094	2.114	2.132	2.136	2.158	2.182	2.206
C_{sat} ($J K^{-1}mol^{-1}$)	209.7	211.8	213.5	213.9	216.2	218.5	220.9
Temp. (K)	340	350	360	370	380		
c_{sat} ($J K^{-1}g^{-1}$)	2.231	2.258	2.286	2.316	2.348		
C_{sat} ($J K^{-1}mol^{-1}$)	223.5	226.2	229.0	232.0	235.2		

TABLE 43.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	44	42	1.213	6.18–2	0.24	2.70–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
220.9–382.6	587.00	–6.69332–1	3.03248	1.90323+1	3.69339–2		II

Name: 3–Hexanone
Formula: $C_6H_{12}O$

CAS–RN: 589–38–8
Group No.: 43–022
Molar Mass: 100.16

TABLE 43.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70AND/COU	222.3–321.7	24	nosp	99.95	melpt	C_{sat}	BSAO	63AND/COU1

TABLE 43.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.328	1.66–2	0.07	1.90–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
222.3–321.7		2.79400+1	–3.89536	1.09711			II

TABLE 43.22.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	2.049	2.057	2.068	2.080	2.094	2.110	2.116
C_{sat} (J K^{-1}mol^{-1})	205.2	206.1	207.1	208.3	209.8	211.4	211.9
Temp. (K)	280	290	298.15	300	310	320	
c_{sat} (J K^{-1}g^{-1})	2.128	2.148	2.165	2.169	2.192	2.217	
C_{sat} (J K^{-1}mol^{-1})	213.1	215.1	216.8	217.2	219.6	222.1	

TABLE 43.22.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.391	1.98–2	0.08	2.58–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
222.3–321.7	582.80	1.33840+1	9.04498	1.46059+1	4.95115		II

Name: 4–Methyl–2–pentanone
Formula: $C_6H_{12}O$

CAS–RN: 108–10–1
Group No.: 43–023
Molar Mass: 100.16

TABLE 43.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC	298.2	1	0.50	not specified		C_p	BSIO	80FUC
89VES/BAR	298.1–318.1	5	0.50	99.97	chrom	C_p	BSAO	79VES/ZAB

TABLE 43.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89VES/BAR	298.1–318.1	5	0.50	0.073	9.47–3	0.04	7.25–6	–1
				Rejected data				
80FUC	(4.63–1, 1.78, 4.63–1, 1)							

TABLE 43.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	5	0.094	1.22–2	0.05	7.25–6	–1

Temp. range K	A_1	A_2	Level of uncertainty
298.1–318.1	1.60928+1	3.15195	III

TABLE 43.23.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	2.095	2.116	2.121	2.147	2.173
C_p ($J\,K^{-1}mol^{-1}$)	209.8	211.9	212.4	215.0	217.7

Name: Benzaldehyde
Formula: C_7H_6O

CAS–RN: 100–52–7
Group No.: 43–024
Molar Mass: 106.12

TABLE 43.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*98LOU	N	370.1	1	nosp	not specified		C_{avg}	DSIO	*98LOU
02LOU1	N	372.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
34KOL/UDO2	N	302.3	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
75AMB/CON		218.0–360.0	39	nosp	99.93	melpt	C_p	BSAO	63AND/COU1
75AMB/CON		325.3–425.3	30	nosp	99.93	melpt	C_p	BSAO	67AND/COU
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC

*98LOU average value in temperature range 295–445 K
02LOU1 average value in temperature range 294–451 K
34KOL/UDO2 same datum in 34KOL/UDO1

TABLE 43.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75AMB/CON	218.0–360.0	39	0.20#	0.506	2.16–2	0.10	9.74–3	12
75AMB/CON	325.3–425.3	30	0.30#	0.735	4.87–2	0.22	–2.82–2	–15
				Rejected data				
*98LOU	(5.23–2, 0.23,–5.23–2, –1)			02LOU1	(7.92–1, 3.33, 7.92–1, 1)			
34KOL/UDO2	(2.16–1, 1.05,–2.16–1, –1)			80FUC	(7.08–1, 3.31, 7.08–1, 1)			

TABLE 43.24.3. Parameters of cubic spline polynomials

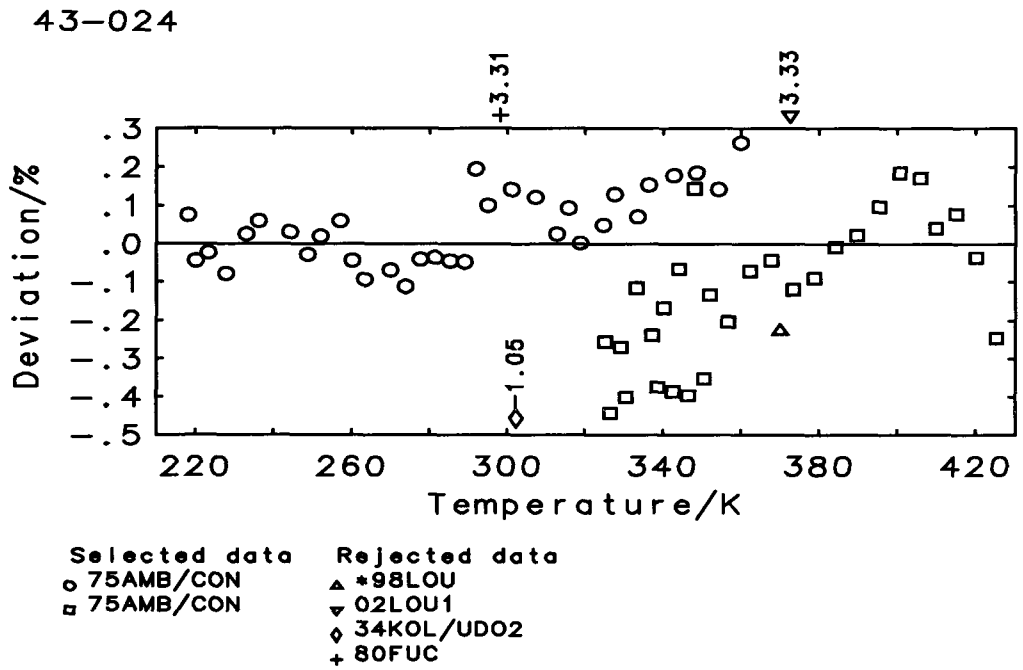
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	73	69	0.640	3.74–2	0.17	–6.74–3	–3
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
218.0–320.0	2.58389+1	–1.01675+1	4.08131	–4.19473–1			II
320.0–425.3	1.02690+1	4.42933	–4.80188–1	5.56828–2			III

TABLE 43.24.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.470	1.484	1.500	1.518	1.537	1.558	1.564
C_p (J K^{-1}mol^{-1})	156.0	157.5	159.2	161.1	163.1	165.3	166.0
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.579	1.602	1.621	1.625	1.649	1.673	1.697
C_p (J K^{-1}mol^{-1})	167.6	170.0	172.0	172.5	175.0	177.5	180.1
Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	1.721	1.745	1.770	1.794	1.819	1.845	1.870
C_p (J K^{-1}mol^{-1})	182.6	185.2	187.8	190.4	193.1	195.7	198.4
Temp. (K)	410	420	430				
c_p (J K^{-1}g^{-1})	1.896	1.922	1.9480				
C_p (J K^{-1}mol^{-1})	201.2	203.9	206.73				

TABLE 43.24.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	73	69	1.168	5.46–2	0.25	2.44–3	15
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
218.0–425.3	695.00	–5.17407	8.81617–1	1.30032+1	7.59146		III



Name: Cycloheptanone
Formula: $C_7H_{12}O$

CAS–RN: 502–42–1
Group No.: 43–025
Molar Mass: 112.17

TABLE 43.25.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC	298.20	1.888	0.50	not specified		C_p	BSIO	80FUC

Name: 2–Methylcyclohexanone
Formula: $C_7H_{12}O$

CAS–RN: 583–60–8
Group No.: 43–026
Molar Mass: 112.17

TABLE 43.26.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.65	1.824	nosp	not specified		C_p	DSIO	22HER/SCH

Name: 3–Methylcyclohexanone
Formula: $C_7H_{12}O$

CAS–RN: 591–24–2
Group No.: 43–027
Molar Mass: 112.17

TABLE 43.27.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.65	1.845	nosp	not specified		C_p	DSIO	22HER/SCH

Name: 4–Methylcyclohexanone
Formula: $C_7H_{12}O$

CAS–RN: 589–92–4
Group No.: 43–028
Molar Mass: 112.17

TABLE 43.28.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24HER/BLO	289.65	1.845	nosp	not specified		C_p	DSIO	22HER/SCH

Name: 3,4–Dimethylpentanal
Formula: $C_7H_{14}O$

CAS–RN: 19353–21–0
Group No.: 43–029
Molar Mass: 114.19

TABLE 43.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87MIL/FEN1	323.1–428.1	22	1.50	99.	chrom	C_p	BDHT	87PER/COM

TABLE 43.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.364	1.79–1	0.55	1.67–3	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
323.1–428.1	8.15673+1	–3.41756+1	5.47174	V

TABLE 43.29.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J\,K^{-1}g^{-1}$)	2.06	2.07	2.08	2.11	2.14	2.19	2.24
C_p ($J\,K^{-1}mol^{-1}$)	235	236	238	241	245	250	255
Temp. (K)	390	400	410	420	430		
c_p ($J\,K^{-1}g^{-1}$)	2.29	2.36	2.43	2.52	2.61		
C_p ($J\,K^{-1}mol^{-1}$)	262	269	278	287	298		

TABLE 43.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.433	2.13–1	0.65	2.29–3	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
323.1–428.1	560.00	1.30530+1	7.54561	1.82265+1	5.64504	V

Name: 2,4–Dimethyl–3–pentanone
Formula: $C_7H_{14}O$

CAS–RN: 565–80–0
Group No.: 43–030
Molar Mass: 114.19

TABLE 43.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70AND/COU	208.1–319.0	23	nosp	99.4	melpt	C_{sat}	BSAO	63AND/COU1

TABLE 43.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.146	7.89–3	0.03	2.82–6	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
208.1–319.0	2.65696+1	–5.17427	2.65229	–2.41601–1	II

TABLE 43.30.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.832	1.853	1.876	1.900	1.925	1.951	1.979
C_{sat} (J K^{-1}mol^{-1})	209.2	211.6	214.2	216.9	219.8	222.8	226.0
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.988	2.008	2.037	2.062	2.068	2.099	2.130
C_{sat} (J K^{-1}mol^{-1})	227.0	229.2	232.6	235.4	236.1	239.6	243.2

TABLE 43.30.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.294	1.57–2	0.06	1.56–5	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
208.1–319.0	575.00	–5.46351	2.29972	1.78509+1	3.24496	II

Name: Heptanal
Formula: $C_7H_{14}O$

CAS–RN: 111–71–7
Group No.: 43–031
Molar Mass: 114.19

TABLE 43.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		359.2–368.0	3S	nosp	not specified		C_{avg}	DSIO	*81VON
56PAR/KEN		230.0–300.0	8S	1.00	96.9	melpt	C_p	BSIO	25PAR
83DYA	N	229.2–350.0	15S	1.00	98.56	melpt	C_p	BSAO	77KU/COM

83DYA error above 1.0 % reported in 84VAS/PET

TABLE 43.31.2. Correlated heat capacities

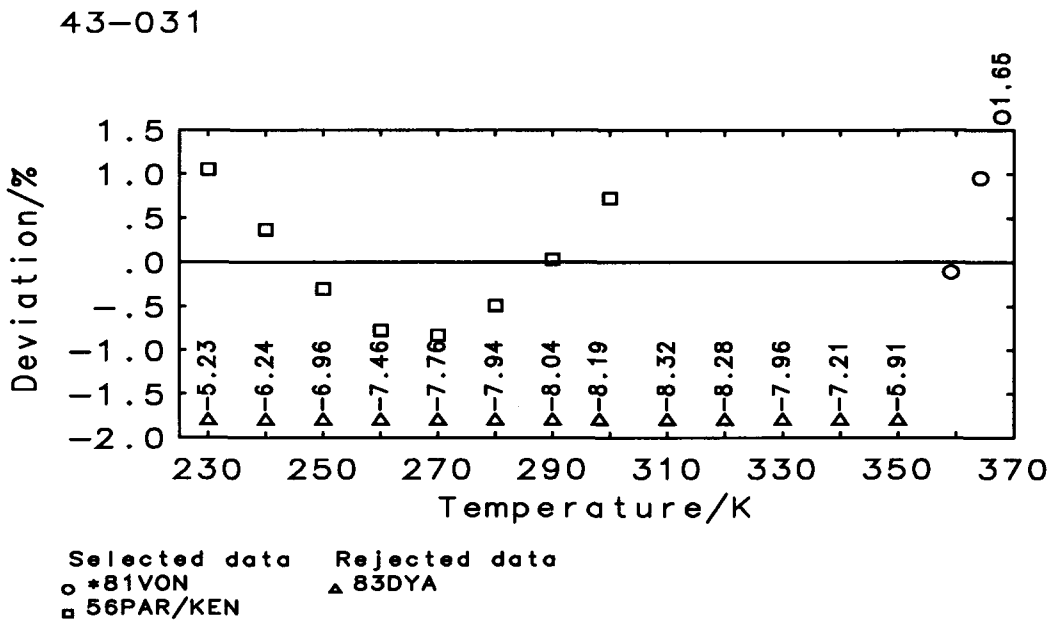
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	359.2–368.0	3	3.00#	0.368	3.59–1	1.10	2.70–1	1
56PAR/KEN	230.0–300.0	8	1.00	0.652	1.88–1	0.65	–8.28–3	0
				Rejected data				
83DYA	(2.07, 7.47,–2.05, –14)							

TABLE 43.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	11	0.650	2.73–1	0.88	6.76–2	1
Temp. range K		A_1	A_2				Level of uncertainty
230.0–368.0		2.08124+1	3.06427				V

TABLE 43.31.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	2.03	2.05	2.07	2.10	2.12	2.12	2.14
C_p (J K^{-1}mol^{-1})	232	234	237	239	242	243	244
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.16	2.18	2.18	2.21	2.23	2.25	2.27
C_p (J K^{-1}mol^{-1})	247	249	249	252	255	257	260
Temp. (K)	350	360	370				
c_p (J K^{-1}g^{-1})	2.30	2.32	2.34				
C_p (J K^{-1}mol^{-1})	262	265	267				



Name: 2–Heptanone
Formula: $C_7H_{14}O$

CAS–RN: 110–43–0
Group No.: 43–032
Molar Mass: 114.19

TABLE 43.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC	298.2–298.2	2	0.50	not specified		C_p	BSIO	80FUC

TABLE 43.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.058	8.50–3	0.03	1.91–6	0

Temp. range K	A_1	Level of uncertainty
298.2–298.2	2.93042+1	V

TABLE 43.32.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.13
C_p (J K^{-1}mol^{-1})	244

Name: 4–Heptanone
Formula: $C_7H_{14}O$

CAS–RN: 123–19–3
Group No.: 43–033
Molar Mass: 114.19

TABLE 43.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*98LOU	N	353.4	1	nosp	not specified		C_{avg}	DSIO	*98LOU
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC

*98LOU average value in temperature range 294–413 K

TABLE 43.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
*98LOU	353.4	1	3.00#	0.000	0.00	0.00	0.00	0
80FUC	298.2	1	0.50	0.000	0.00	0.00	0.00	0

TABLE 43.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
298.2–353.4	1.83021+1	3.79639	V

TABLE 43.33.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p (J K^{-1}g^{-1})	2.16	2.19	2.22	2.24	2.27	2.30
C_p (J K^{-1}mol^{-1})	247	250	253	256	259	263

Name: 3–Methylhexanal
Formula: $C_7H_{14}O$

CAS–RN: 19269–28–4
Group No.: 43–034
Molar Mass: 114.19

TABLE 43.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87MIL/FEN1	323.1–428.1	22	1.50	99.	chrom	C_p	BDHT	87PER/COM

TABLE 43.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.200	9.57–2	0.30	4.85–4	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
323.1–428.1	2.59552+2	–1.86490+2	4.89406+1	–4.09992	V

TABLE 43.34.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.15	2.17	2.19	2.23	2.27	2.32	2.38
C_p (J K^{-1}mol^{-1})	246	247	250	254	259	265	271
Temp. (K)	390	400	410	420	430		
c_p (J K^{-1}g^{-1})	2.43	2.49	2.55	2.61	2.66		
C_p (J K^{-1}mol^{-1})	278	285	292	298	304		

TABLE 43.34.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.351	1.73–1	0.53	1.54–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
323.1–428.1	595.20	–4.10386	3.75100	1.73255+1	1.12247	V

Name: 2–Methyl–3–hexanone
Formula: $C_7H_{14}O$

CAS–RN: 7379–12–6
Group No.: 43–035
Molar Mass: 114.19

TABLE 43.35.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80FUC	298.20	2.115	0.50	not specified		C_p	BSIO	80FUC

Name: 1–Phenylethanone
Formula: C_8H_8O

CAS–RN: 98–86–2
Group No.: 43–036
Molar Mass: 120.15

TABLE 43.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
00LOU	N	381.1	1	nosp	not specified		C_{avg}	DSIO	*98LOU
39PHI		303.1	1	nosp	not specified		C_p	BSIO	49WEI
80FUC		298.2–298.2	2	0.50	not specified		C_p	BSIO	80FUC

00LOU average value in temperature range 293–469 K

TABLE 43.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
00LOU	381.1	1	3.00#	0.000	0.00	0.00	0.00	0
80FUC	298.2	2	0.50	0.439	5.41–2	0.22	2.36–4	0
				Rejected data				
39PHI	(2.49, 9.08, 2.49, 1)							

TABLE 43.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	3	0.621	7.65–2	0.31	1.58–4	0

Temp. range K	A_1	A_2	Level of uncertainty
298.2–381.1	1.02038+1	4.84832	V

TABLE 43.36.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.71	1.75	1.78	1.81	1.85	1.88	1.91
C_p (J K^{-1}mol^{-1})	206	210	214	218	222	226	230
Temp. (K)	370	380					
c_p (J K^{-1}g^{-1})	1.95	1.98					
C_p (J K^{-1}mol^{-1})	234	238					

Name: 6–Methyl–5–hepten–2–one
Formula: $C_8H_{14}O$

CAS–RN: 110–93–0
Group No.: 43–037
Molar Mass: 126.20

TABLE 43.37.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84BAG/BAE	N	273.4–343.4	4	0.80	99.0	estim	C_p	BDHT	86CDA/COM

84BAG/BAE same data in 86BER/GUR and 88BAG/GUR

TABLE 43.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	1.067	2.82–1	0.85	2.34–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
273.4–343.4		2.36268+1	2.90097				V

TABLE 43.37.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.07	2.08	2.09	2.11	2.13	2.13	2.15
C_p (J K^{-1}mol^{-1})	262	262	264	266	268	269	271
Temp. (K)	320	330	340				
c_p (J K^{-1}g^{-1})	2.17	2.19	2.21				
C_p (J K^{-1}mol^{-1})	274	276	278				

Name: Octanal
Formula: $C_8H_{16}O$

CAS–RN: 124–13–0
Group No.: 43–038
Molar Mass: 128.21

TABLE 43.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83DYA	N	247.7–350.0	13S	nosp	not specified		C_p	BSAO	77KU/COM

83DYA error above 1.0 % reported in 84VAS/PET

TABLE 43.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.092	5.59–2	0.18	1.47–4	–5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
247.7–350.0		–3.64691+1	6.62057+1	–2.25225+1	2.66095		V

TABLE 43.38.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.94	1.96	1.98	1.98	1.99	2.01	2.03
C_p (J K^{-1}mol^{-1})	248	251	253	254	256	258	260
Temp. (K)	300	310	320	330	340	350	
c_p (J K^{-1}g^{-1})	2.03	2.05	2.07	2.10	2.13	2.17	
C_p (J K^{-1}mol^{-1})	260	263	266	269	273	278	

TABLE 43.38.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.130	8.21–2	0.26	3.34–4	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
247.7–350.0	617.00	5.92834	8.20847	1.87464+1	1.07040		V

Name: 2–Octanone
Formula: $C_8H_{16}O$

CAS–RN: 111–13–7
Group No.: 43–039
Molar Mass: 128.21

TABLE 43.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		324.7–380.3	5S	nosp	not specified		C_{avg}	DSIO	*81VON
*98LOU	N	367.8	1	nosp	not specified		C_{avg}	DSIO	*98LOU
02LOU1	N	370.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
65OET		257.8–333.2	29	0.30	99.68	melpt	C_{sat}	BSAO	58HIL/KRA
80FUC		298.2	1	0.50	not specified		C_p	BSIO	80FUC

*98LOU average value in temperature range 294–441 K
02LOU1 average value in temperature range 296–445 K

TABLE 43.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	324.7–380.3	5	2.00#	0.132	9.20–2	0.26	–2.91–2	–3
*98LOU	367.8	1	3.00#	0.016	1.71–2	0.05	1.71–2	1
65OET	257.8–333.2	29	0.30	0.333	3.27–2	0.10	1.69–4	–1
				Rejected data				
02LOU1	(1.20, 3.24, 1.20, 1)			80FUC	(4.33–1, 1.30, 4.33–1, 1)			

TABLE 43.39.3. Parameters of regression polynomial

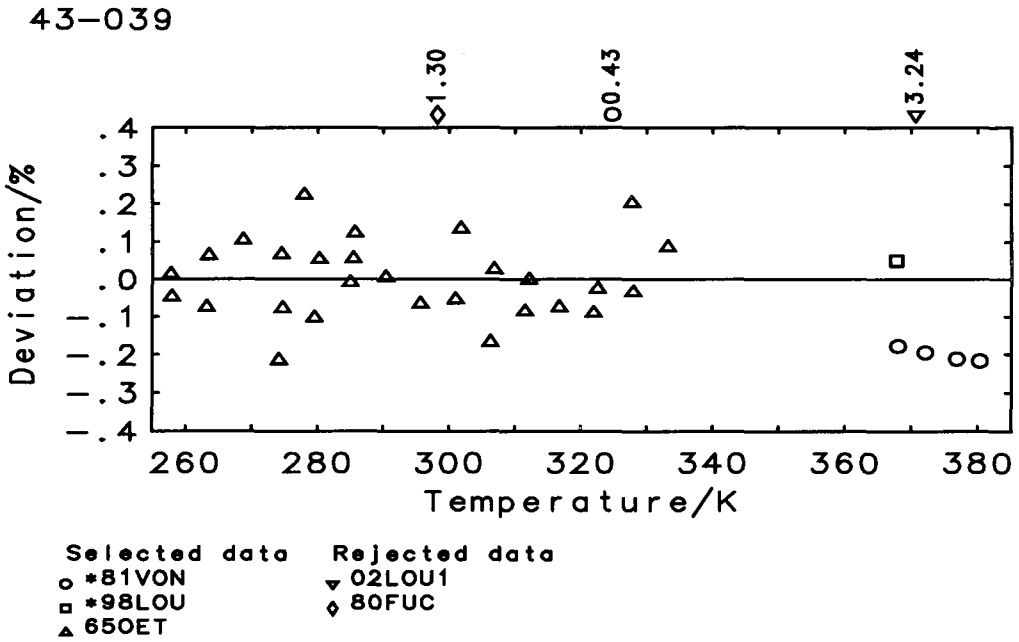
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	37	35	0.326	4.87–2	0.14	–3.53–3	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
257.8–380.3		6.46831+1	–3.48811+1	1.14806+1	–1.12706		III

TABLE 43.39.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	2.062	2.076	2.081	2.093	2.114	2.131	2.136
C_{sat} (J K^{-1}mol^{-1})	264.3	266.2	266.8	268.4	271.0	273.3	273.8
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	2.160	2.185	2.211	2.238	2.264	2.290	2.315
C_{sat} (J K^{-1}mol^{-1})	276.9	280.1	283.5	286.9	290.3	293.6	296.9
Temp. (K)	380						
c_{sat} (J K^{-1}g^{-1})	2.339						
C_{sat} (J K^{-1}mol^{-1})	299.9						

TABLE 43.39.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	37	35	0.803	8.48–2	0.26	2.20–2	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
257.8–380.3	623.80	–4.67759	4.86234–1	2.35616+1	1.12497+1		III



Name: 3–Phenyl–2–propenal
Formula: C_9H_8O

CAS–RN: 104–55–2
Group No.: 43–040
Molar Mass: 132.16

TABLE 43.40.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC	298.20	1.760	0.50	not specified		C_p	BSIO	80FUC

Name: 1–Phenyl–1–propanone
Formula: $C_9H_{10}O$

CAS–RN: 93–55–0
Group No.: 43–041
Molar Mass: 134.18

TABLE 43.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC	298.2–298.2	3	0.50	not specified		C_p	BSIO	80FUC

TABLE 43.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.342	5.01–2	0.17	1.15–4	1
Temp. range K		A_1					Level of uncertainty
298.2–298.2		2.93061+1					V

TABLE 43.41.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	1.82
C_p (J K^{-1}mol^{-1})	244

Name: 2,5,6–Trimethyl–2–cyclohexen–1–one
Formula: $C_9H_{14}O$

CAS–RN: 20030–30–2
Group No.: 43–042
Molar Mass: 138.21

TABLE 43.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.3–343.5	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 84BAG/BAE and 88BAG/GUR

TABLE 43.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.337	2.10–1	0.67	1.57–3	0

Temp. range K	A_1	A_2	Level of uncertainty
273.3–343.5	1.75733+1	4.61056	V

TABLE 43.42.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.81	1.81	1.83	1.86	1.88	1.89	1.92
C_p (J K^{-1}mol^{-1})	250	251	253	257	260	261	265

Temp. (K)	320	330	340
c_p (J K^{-1}g^{-1})	1.94	1.97	2.00
C_p (J K^{-1}mol^{-1})	269	273	276

Name: 2,6–Dimethyl–4–heptanone
Formula: $C_9H_{18}O$

CAS–RN: 108–83–8
Group No.: 43–043
Molar Mass: 142.24

TABLE 43.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89VES/BAR	298.1–318.1	5	0.50	99.99	chrom	C_p	BSAO	79VES/ZAB

TABLE 43.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.176	3.17–2	0.09	3.13–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–318.1		1.99981+1	5.29660				III

TABLE 43.43.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	2.067	2.092	2.098	2.129	2.160
C_p (J K^{-1}mol^{-1})	294.0	297.6	298.4	302.8	307.2

Name: Nonanal
Formula: $C_9H_{18}O$

CAS–RN: 124–19–6
Group No.: 43–044
Molar Mass: 142.24

TABLE 43.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DYA	N	253.8–340.0	21S	1.00	99.00	melpt	C_p	BSAO	77KU/COM

83DYA error above 1.0 % reported in 84VAS/PET

TABLE 43.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	21	0.231	7.87–2	0.23	2.73–4	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
253.8–340.0		–1.33429+2	1.61413+2	–5.23060+1	5.73947		V

TABLE 43.44.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.96	1.99	2.00	2.01	2.03	2.04	2.05
C_p (J K^{-1}mol^{-1})	279	283	284	286	289	291	291
Temp. (K)	310	320	330	340			
c_p (J K^{-1}g^{-1})	2.06	2.08	2.10	2.12			
C_p (J K^{-1}mol^{-1})	293	296	298	302			

TABLE 43.44.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	21	0.320	1.11–1	0.32	6.05–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
253.8–340.0	640.00	8.75875+1	1.41897+1	4.23245–1	1.35161+2		V

Name: 5–Nonanone
Formula: $C_9H_{18}O$

CAS–RN: 502–56–7
Group No.: 43–045
Molar Mass: 142.24

TABLE 43.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70AND/COU	277.2–320.0	10	nosp	99.85	melpt	C_{sat}	BSAO	63AND/COU1
79SAL/PEA	298.1–298.1	2	nosp	not specified		C_p	BSIO	80FUC
80FUC	298.2	1	0.50	not specified		C_p	BSIO	80FUC

TABLE 43.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70AND/COU	277.2–320.0	10	0.20#	0.152	1.12–2	0.03	4.96–6	–1
				Rejected data				
79SAL/PEA	(3.55–1, 0.96, 3.47–1, 2)			80FUC	(4.19–1, 1.14, 4.19–1, 1)			

TABLE 43.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	13	10	0.182	1.34–2	0.04	4.96–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
277.2–320.0		4.27398+1	–7.87577	1.94120			II

TABLE 43.45.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	2.099	2.118	2.134	2.138	2.162	2.187
C_{sat} (J K^{-1}mol^{-1})	298.5	301.2	303.6	304.2	307.5	311.1

Name: 1–(4–Ethylphenyl)ethanone
Formula: $C_{10}H_{12}O$

CAS–RN: 937–30–4
Group No.: 43–046
Molar Mass: 148.20

TABLE 43.46.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80FUC	298.20	1.759	0.50	not specified		C_p	BSIO	80FUC

Name: Camphor
Formula: $C_{10}H_{16}O$

CAS–RN: 76–22–2
Group No.: 43–047
Molar Mass: 152.24

TABLE 43.47.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31FRA	N	451.5–483.1	2	8.00	not specified		C_{sat}	DSIO	26AND/LYN

31FRA constant value calculated from temperature dependence of enthalpy by the authors

TABLE 43.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
451.5–483.1	4.37431+1	VI

TABLE 43.47.4. Recommended values of heat capacities

Temp. (K)	450	460	470	480
c_{sat} (J $K^{-1}g^{-1}$)	2.39	2.39	2.39	2.39
C_{sat} (J $K^{-1}mol^{-1}$)	364	364	364	364

Name: 3,7,–Dimethyl–2,6–octadienal
Formula: $C_{10}H_{16}O$

CAS–RN: 5392–40–5
Group No.: 43–048
Molar Mass: 152.24

TABLE 43.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82KAR/IGA	233.0–293.0	4S	0.30	not specified		C_p	BSAO	82KAR/IGA

TABLE 43.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.603	6.15–2	0.18	4.72–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
233.0–293.0		3.22401+1	–7.03312	2.91236			IV

TABLE 43.48.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.719	1.755	1.795	1.837	1.883	1.898	1.932
C_p (J K^{-1}mol^{-1})	261.7	267.2	273.2	279.7	286.7	289.0	294.2
Temp. (K)	290	298.15					
c_p (J K^{-1}g^{-1})	1.985	2.030					
C_p (J K^{-1}mol^{-1})	302.1	309.0					

Name: 5–Methyl–2–(1–methylethylidene)cyclohexanone
Formula: $C_{10}H_{16}O$

CAS–RN: 15932–80–6
Group No.: 43–049
Molar Mass: 152.24

TABLE 43.49.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
33KOL/UDO	N	293.33	1.806	nosp	not specified		C_p	BSIT	34KOL/UDO2

33KOL/UDO same datum in 34KOL/UDO2

Name: Decanal
Formula: $C_{10}H_{20}O$

CAS–RN: 112–31–2
Group No.: 43–050
Molar Mass: 156.27

TABLE 43.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DYA	N	269.3–337.5	21S	1.00	not specified		C_p	BSAO	77KU/COM

83DYA error above 1.0 % reported in 84VAS/PET

TABLE 43.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	21	0.535	2.05–1	0.53	1.68–3	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
269.3–337.5		–4.40579+2	4.66036+2	–1.52077+2	1.66427+1		V

TABLE 43.50.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	1.95	1.96	1.99	2.01	2.03	2.03	2.05
C_p ($J K^{-1} mol^{-1}$)	305	307	311	315	317	318	320
Temp. (K)	320	330	340				
c_p ($J K^{-1} g^{-1}$)	2.07	2.09	2.13				
C_p ($J K^{-1} mol^{-1}$)	323	327	333				

Name: Diphenyl methanone
Formula: $C_{13}H_{10}O$

CAS–RN: 119–61–9
Group No.: 43–051
Molar Mass: 182.22

TABLE 43.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83DEK/VAN	322.5–346.6	22	nosp	99.53	melpt	C_p	BSAO	79SCH/OFF

TABLE 43.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.053	1.32–2	0.04	7.63–6	5
Temp. range K		A_1	A_2				Level of uncertainty
322.5–346.6		1.77926+1	5.58497				IV

TABLE 43.51.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.653	1.678	1.704
C_p ($J K^{-1} mol^{-1}$)	301.2	305.8	310.5

Name: 6,10–Dimethyl–3,5,9–undecatriene–2–one
Formula: $C_{13}H_{20}O$

CAS–RN: 141–10–6
Group No.: 43–052
Molar Mass: 192.30

TABLE 43.52.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.3–343.4	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 43.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.369	3.43–1	0.74	2.55–3	0
Temp. range K		A_1	A_2				Level of uncertainty
273.3–343.4		3.17649+1	4.90046				V

TABLE 43.52.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.95	1.95	1.97	1.99	2.01	2.01	2.03
C_p (J K^{-1}mol^{-1})	374	375	378	382	386	386	390
Temp. (K)	320	330	340				
c_p (J K^{-1}g^{-1})	2.05	2.07	2.09				
C_p (J K^{-1}mol^{-1})	394	399	403				

Name: 6,10–Dimethyl–4,5,9–undecatriene–2–one
Formula: $C_{13}H_{20}O$

CAS–RN: 16647–05–5
Group No.: 43–053
Molar Mass: 192.30

TABLE 43.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	%	Purity method	Type capacity	Calorimeter Type	Reference
86BER/GUR	N	273.0–333.8	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 43.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.201	1.99–1	0.40	7.52–4	0
Temp. range K		A_1	A_2				Level of uncertainty
273.0–333.8		2.61292+1	7.46512				V

TABLE 43.53.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.00	2.01	2.03	2.07	2.09	2.10	2.13
C_p (J K^{-1}mol^{-1})	385	387	391	397	402	403	410
Temp. (K)	320	330					
c_p (J K^{-1}g^{-1})	2.16	2.19					
C_p (J K^{-1}mol^{-1})	416	422					

Name: 4–(2,6,6–Trimethyl–1–cyclohexen–1–yl)–3–buten–2–one
Formula: $C_{13}H_{20}O$

CAS–RN: 14901–07–6
Group No.: 43–054
Molar Mass: 192.30

TABLE 43.54.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.2–333.8	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 43.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.313	2.92–1	0.63	1.71–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
273.2–333.8		2.71798+1	6.10234				V

TABLE 43.54.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.89	1.90	1.91	1.94	1.96	1.97	1.99
C_p ($J\,K^{-1}mol^{-1}$)	363	365	368	373	377	378	383
Temp. (K)	320	330					
c_p ($J\,K^{-1}g^{-1}$)	2.02	2.05					
C_p ($J\,K^{-1}mol^{-1}$)	388	393					

Name: 6,10–Dimethyl–2–undecanone
Formula: $C_{13}H_{26}O$

CAS–RN: 1604–34–8
Group No.: 43–055
Molar Mass: 198.35

TABLE 43.55.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.0–343.4	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 43.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.172	1.76–1	0.34	8.11–4	0
Temp. range K		A_1	A_2				Level of uncertainty
273.0–343.4		2.41730+1	8.80587				V

TABLE 43.55.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	2.01	2.02	2.05	2.08	2.11	2.12	2.16
C_p ($J K^{-1}mol^{-1}$)	399	401	406	413	419	421	428
Temp. (K)	320	330	340				
c_p ($J K^{-1}g^{-1}$)	2.19	2.23	2.27				
C_p ($J K^{-1}mol^{-1}$)	435	443	450				

Name: 9,10–Anthracenedione
Formula: $C_{14}H_8O_2$

CAS–RN: 84–65–1
Group No.: 43–056
Molar Mass: 208.22

TABLE 43.56.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	%	Purity method	Type capacity	Calorimeter Type	Reference
17HIL/DUS	N	573.15	2.761	nosp	not specified		C_{avg}	DSIO	11LEW/RAN

17HIL/DUS average value in temperature range 558–593 K

Name: (3–Methylphenyl)phenylmethanone
Formula: $C_{14}H_{12}O$

CAS–RN: 643–65–2
Group No.: 43–057
Molar Mass: 196.25

TABLE 43.57.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	%	Purity method	Type capacity	Calorimeter Type	Reference
80FUC	298.20	1.657	0.50	not specified		C_p	BSIO	80FUC

Name: 2–(1,2–Dimethylpropyl)–5,6–dimethyl–2–heptenal
Formula: $C_{14}H_{26}O$

CAS–RN: 99914–84–8
Group No.: 43–058
Molar Mass: 210.36

TABLE 43.58.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	%	Purity method	Type capacity	Calorimeter Type	Reference
87MIL/FEN2	323.1–428.1	22	1.50	98.	chrom	C_p	BDHT	87PER/COM

TABLE 43.58.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.227	1.87–1	0.34	1.06–3	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
323.1–428.1		4.11992+2	–3.01348+2	8.14054+1	–7.04381		V

TABLE 43.58.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.99	2.01	2.04	2.07	2.12	2.16	2.21
C_p (J K^{-1}mol^{-1})	420	423	429	436	445	454	464
Temp. (K)	390	400	410	420	430		
c_p (J K^{-1}g^{-1})	2.26	2.30	2.35	2.39	2.42		
C_p (J K^{-1}mol^{-1})	475	485	494	503	510		

TABLE 43.58.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.329	2.71–1	0.49	2.30–3	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
323.1–428.1	707.00	–1.65819+1	6.50787	2.32592+1	1.05626+1		V

Name: 2–Pentyl–2–nonenal
Formula: $C_{14}H_{26}O$

CAS–RN: 3021–89–4
Group No.: 43–059
Molar Mass: 210.36

TABLE 43.59.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
87MIL/FEN2	323.1–428.1	22	1.50	99.	chrom	C_p	BDHT	87PER/COM

TABLE 43.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.556	4.70–1	0.83	6.89–3	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
323.1–428.1		8.92636+2	–6.80078+2	1.80682+2	–1.56754+1		V

TABLE 43.59.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.09	2.08	2.09	2.12	2.16	2.21	2.26
C_p (J K^{-1}mol^{-1})	440	438	440	446	454	465	476
Temp. (K)	390	400	410	420	430		
c_p (J K^{-1}g^{-1})	2.32	2.37	2.42	2.46	2.48		
C_p (J K^{-1}mol^{-1})	488	499	509	517	522		

TABLE 43.59.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	22	0.759	6.68–1	1.14	1.30–2	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
323.1–428.1	718.00	1.91970+1	2.58484+1	1.47851+1	3.56429	V

Name: 2–Tetradecanone
Formula: $C_{14}H_{28}O$

CAS–RN: 2345–27–9
Group No.: 43–060
Molar Mass: 212.38

TABLE 43.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79SUN/SVE	313.0–338.0	eqn	nosp	99.93	chrom	C_p	BDHT	69PER/COM

TABLE 43.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	3.30–6	0.00	–6.36–7	0

Temp. range K	A_1	A_2	Level of uncertainty
313.0–338.0	3.83892+1	5.77305	V

TABLE 43.60.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	2.20	2.23	2.25	2.27
C_p ($J\,K^{-1}mol^{-1}$)	468	473	478	482

Name: 2–Pentadecanone
Formula: $C_{15}H_{30}O$

CAS–RN: 2345–28–0
Group No.: 43–061
Molar Mass: 226.40

TABLE 43.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79SUN/SVE	318.0–343.0	eqn	nosp	99.96	chrom	C_p	BDHT	69PER/COM

TABLE 43.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.000	2.20–6	0.00	9.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
318.0–343.2		4.20913+1	5.80912				V

TABLE 43.61.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c_p ($J K^{-1}g^{-1}$)	2.23	2.25	2.27
C_p ($J K^{-1}mol^{-1}$)	505	509	514

Name: 1,4–Diphenyl–1,4–butanedione
Formula: $C_{16}H_{14}O_2$

CAS–RN: 495–71–6
Group No.: 43–062
Molar Mass: 238.29

TABLE 43.62.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
32SPA/THO	423.1–463.1	5S	1.00	not specified		C_p	BDHO	31THO/PAR

TABLE 43.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	4.40–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
423.1–463.1		4.54522+1	3.59730				V

TABLE 43.62.4. Recommended values of heat capacities

Temp. (K)	430	440	450	460
c_p ($J K^{-1}g^{-1}$)	2.13	2.14	2.15	2.16
C_p ($J K^{-1}mol^{-1}$)	507	510	513	515

Name: 6,10,14–Trimethyl–3,5–pentadecadien–2–one
Formula: $C_{18}H_{32}O$

CAS–RN: 1604–32–6
Group No.: 43–063
Molar Mass: 264.45

TABLE 43.63.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.4–333.5	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 43.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.431	5.89–1	0.86	5.26–3	2
Temp. range K		A_1	A_2				Level of uncertainty
273.4–333.5		4.03670+1	8.91640				V

TABLE 43.63.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.03	2.03	2.05	2.08	2.10	2.11	2.14
C_p (J K^{-1}mol^{-1})	536	538	543	551	557	558	565
Temp. (K)	320	330					
c_p (J K^{-1}g^{-1})	2.17	2.19					
C_p (J K^{-1}mol^{-1})	573	580					

Name: 6,10,14–Trimethyl–2–pentadecanone
Formula: $C_{18}H_{36}O$

CAS–RN: 502–69–2
Group No.: 43–064
Molar Mass: 268.48

TABLE 43.64.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.0–333.6	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 43.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.371	5.32–1	0.74	4.21–3	2
Temp. range K		A_1	A_2				Level of uncertainty
273.0–333.6		3.03818+1	1.41765+1				V

TABLE 43.64.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	2.13	2.14	2.17	2.21	2.25	2.26	2.30
C_p ($J\,K^{-1}mol^{-1}$)	571	575	583	594	604	606	618
Temp. (K)	320	330					
c_p ($J\,K^{-1}g^{-1}$)	2.35	2.39					
C_p ($J\,K^{-1}mol^{-1}$)	630	642					

44. Acids and Anhydrides

This family contains 36 compounds of which three were measured at one temperature only.

Data over a wide temperature range are available for three acids only (acetic, propanoic and butanoic acids) and were studied at NPLT (82MAR/AND) using two different adiabatic calorimeters; the recommended data are based exclusively on the NPLT experimental values. The largest number of fatty acids (C_7 to C_{20} fatty acids), and also maleic anhydride, was investigated at SUU (82SCH/VAN1, 82SCH/VAN2) over a limited temperature interval and yielded data with an uncertainty of around 0.5 %. These data were the basis for generating the recommended values; additional experimental data were available for C_{16} and C_{18} acids from the laboratories of the U.S. Department of Agriculture (50SIN/WAR, 52WAR/SIN), but have not been used because of their lower reliability. The data for maleic anhydride were obtained at SUU using two different instruments (adiabatic calorimeter 83DEW/DEK and a DSC device 83DEW/OFF) with the results differing by 10 %. Only the first source has been considered in producing the recommended values.

For some acids and anhydrides, only very old measurements are available having large uncertainties (German sources, *81VON, *86SCH, or data from YUNH, 26AND/LYN). However, these data were considered because no other more recent results were available. In some cases, these data served to extend the temperature range of our recommendations.

Industrially important propenoic acid and 2-methylpropenoic acids (acrylic and methacrylic acids) were studied in the fSU at the Uzbek Academy of Sciences (83KAR/ABD2, 85KAR/ABD1, 85KAR/ABD2) and data were obtained with a claimed error below 0.5 % which does not seem to be a realistic estimate. Although no comparison is possible for propenoic acid, the results for 2-methylpropenoic acid differ by 2 to 3 % from the two data points determined at CIUG (67RAB/LEV) with a probable error of 0.5 %.

The only data available for pyromellitic anhydride are from RAB (78MAR/CIO2) but have been rejected from the correlation. This source is considered to be quite doubtful because the data reported in the same paper for maleic anhydride differed from the values measured at SUU (83DEW/DEK) by more than 40 %.

Name: Formic acid
Formula: CH_2O_2

CAS–RN: 64–18–6
Group No.: 44–001
Molar Mass: 46.03

TABLE 44.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		313.2–341.7	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*86LUD	N	306.1	1	nosp	not specified		C_{avg}	DSIO	*86LUD
*86SCH		309.8–322.7	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
*95MAS/GUI	N	323.1	1	nosp	not specified		C_{avg}	not specified	
20GIB/LAT		286.0–291.5	3	nosp	not specified		C_p	BSIO	20GIB/LAT
34RAD/JUL		290.1	1	nosp	not specified		C_p	BSIO	49WEI
36GLA/CHE		298.1	1	0.50	not specified		C_p	BSIO	32NEU
41STO/FIS	N	275.3–299.8	9	0.20	99.994	melpt	C_p	BSIO	28GIA/WIE1
81CAS/WIL		298.1	1	nosp	99.	melpt	C_p	FSIT	71PIC/LED

*86LUD average value in temperature range 289–323 K
*95MAS/GUI average value in temperature range 293–353 K; calorimeter not identified,probably drop
41STO/FIS experimental temperature multiplied by the factor 273.15/273.10

TABLE 44.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	313.2–341.7	4	2.00#	0.221	5.34–2	0.44	1.13–3	0
41STO/FIS	275.3–299.8	9	0.20	0.703	1.67–2	0.14	4.36–5	1
				Rejected data				
*86LUD	(4.40–1, 3.54, 4.40–1, 1)			*86SCH	(2.13–1, 1.73, 2.01–1, 6)			
*95MAS/GUI	(1.01–1, 0.85,–1.01–1, –1)			20GIB/LAT	(1.09–1, 0.92, –3.45–2, –1)			
34RAD/JUL	(1.39–1, 1.15, 1.39–1, 1)			36GLA/CHE	(1.29–1, 1.09, –1.29–1, –1)			
81CAS/WIL	(1.42–1, 1.18, 1.42–1, 1)							

TABLE 44.1.3. Parameters of regression polynomial

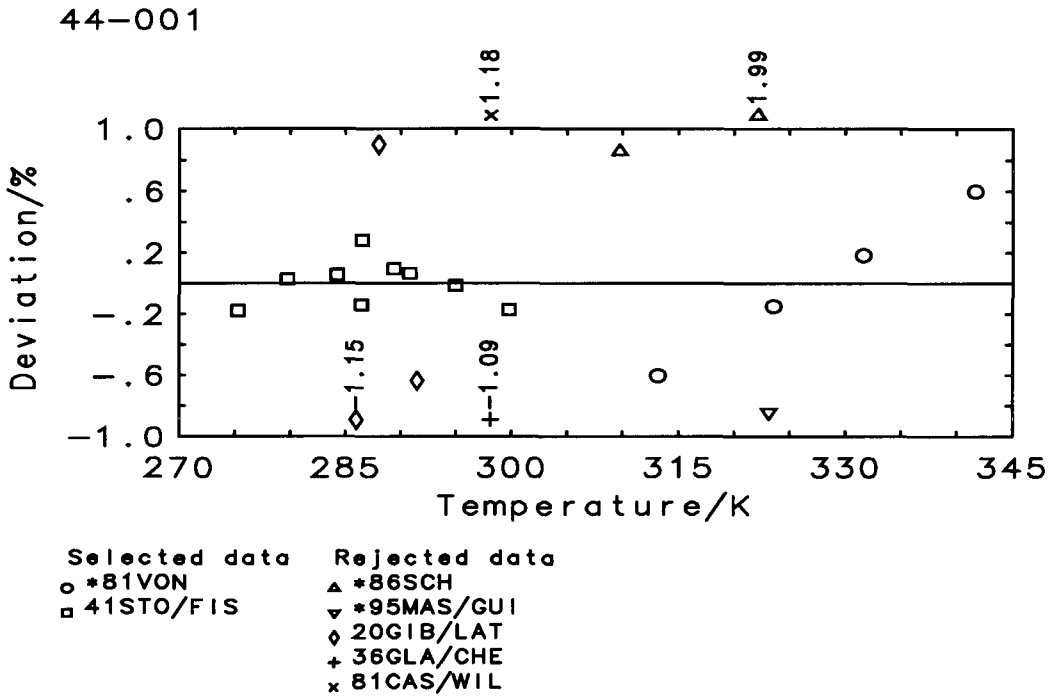
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	13	0.650	3.56–2	0.29	3.77–4	1
Temp. range K		A_1	A_2				Level of uncertainty
275.3–341.7		1.01557+1	5.94119–1				IV

TABLE 44.1.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J $K^{-1}g^{-1}$)	2.135	2.146	2.155	2.157	2.167	2.178	2.189
C_p (J $K^{-1}mol^{-1}$)	98.27	98.76	99.17	99.26	99.75	100.2	100.7
Temp. (K)	340						
c_p (J $K^{-1}g^{-1}$)	2.200						
C_p (J $K^{-1}mol^{-1}$)	101.2						

TABLE 44.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	27	13	1.717	4.22–2	0.36	–1.76–2	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
275.3–341.7	588.00	8.40096+1	2.38733+1	–1.45711+1	7.39070+1		IV



Name: Acetic acid
Formula: $C_2H_4O_2$

CAS–RN: 64–19–7
Group No.: 44–002
Molar Mass: 60.05

TABLE 44.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON		313.5–325.1	3S	nosp	not specified	C_{avg}	DSIO	*81VON
*86LUD	N	308.1	1	nosp	not specified	C_{avg}	DSIO	*86LUD
*86SCH		312.9–337.4	8S	nosp	not specified	C_{avg}	DSIO	*86SCH
*95PIC	N	314.1	1	3.70	not specified	C_{avg}	BDHO	*90PIC
00LOU	N	340.1	1	nosp	not specified	C_{avg}	DSIO	*98LOU
12BAU		290.1	1	nosp	not specified	C_p	not specified	
25PAR/KEL		292.6–294.7	2	nosp	99.9 estim	C_p	BSIO	25PAR
32NEU	N	297.0–353.6	4	nosp	not specified	C_p	BSIO	32NEU
34RAD/JUL		289.6	1	nosp	not specified	C_p	BSIO	49WEI
47PUS/FED		296.4–309.6	6	nosp	not specified	C_p	DSIO	47PUS/FED
58SWI/ZIE1	N	332.3–348.8	2	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
65CAM/GIE		298.6	1	0.50	not specified	C_p	DSIO	64CAM/NAG
81CAS/WIL		298.1	1	nosp	99.8 melpt	C_p	FSIT	71PIC/LED
82MAR/AND		293.2–350.8	30	nosp	99.95 melpt	C_p	BSAO	68WES/FUR
82MAR/AND		315.1–400.2	18	nosp	99.95 melpt	C_p	BSAO	68WES/FUR

*86LUD average value in temperature range 293–323 K
*95PIC average value in temperature range 290–339 K
00LOU average value in temperature range 296–385 K
32NEU same data in 32NEI
58SWI/ZIE1 average values in temperature ranges 295–369 K and 295–402 K

TABLE 44.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
65CAM/GIE	298.6	1	0.50	0.203	1.50–2	0.10	−1.50–2	−1
82MAR/AND	293.2–350.8	30	0.10#	0.264	4.08–3	0.03	9.63–4	4
82MAR/AND	315.1–400.2	18	0.20#	0.516	1.70–2	0.10	−6.24–3	−11
				Rejected data				
*81VON	(1.70–1, 1.10, 1.69–1, 3)			*86LUD	(3.72–1, 2.40, 3.72–1, 1)			
*86SCH	(1.56–1, 0.97, 1.08–1, 4)			*95PIC	(1.17, 7.09, 1.17, 1)			
00LOU	(5.35–2, 0.33, 5.35–2, 1)			25PAR/KEL	(1.27–1, 0.86, 1.27–1, 1)			
32NEU	(2.35–1, 1.52,–2.34–1, −4)			47PUS/FED	(1.52–1, 1.03,–1.51–1, −6)			
58SWI/ZIE1	(7.28–1, 4.34, 6.18–1, 2)			81CAS/WIL	(1.22–1, 0.83, −1.22–1, −1)			

TABLE 44.2.3. Parameters of regression polynomial

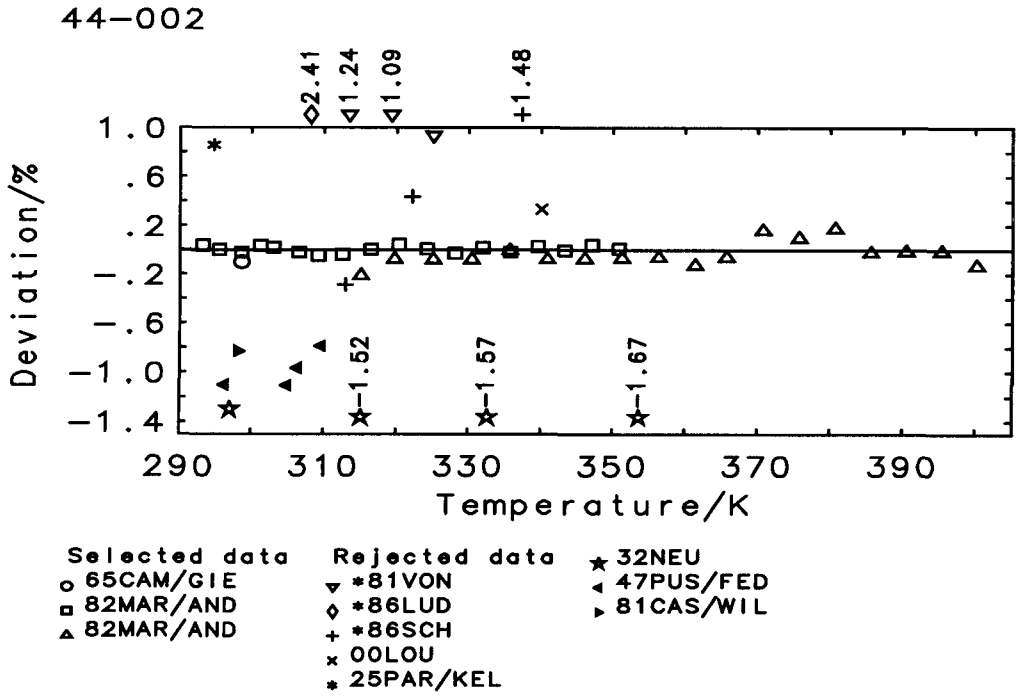
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	80	49	0.388	1.14–2	0.07	−2.01–3	−8
Temp. range K		A_1	A_2	A_3			Level of uncertainty
293.2–400.2		7.94190	1.76406	1.80768–1			II

TABLE 44.2.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.018	2.050	2.058	2.097	2.137	2.178	2.219
C_p (J K^{-1}mol^{-1})	121.2	123.1	123.6	125.9	128.4	130.8	133.3
Temp. (K)	350	360	370	380	390	400	
c_p (J K^{-1}g^{-1})	2.261	2.303	2.346	2.389	2.433	2.477	
C_p (J K^{-1}mol^{-1})	135.8	138.3	140.9	143.5	146.1	148.7	

TABLE 44.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	80	49	0.433	1.17–2	0.07	5.77–4	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
293.2–400.2	592.71	−1.95201	7.49991–2	6.90022	1.27012+1		II



Name: 2–Propenoic acid
Formula: $C_3H_4O_2$

CAS–RN: 79–10–7
Group No.: 44–003
Molar Mass: 72.06

TABLE 44.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83KAR/ABD2		289.3–342.9	21	0.50	not specified		C_p	BSAO	82KAR/IGA
85KAR/ABD1	N	286.0–333.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD1 same data in 85KAR/SAI

TABLE 44.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83KAR/ABD2	289.3–342.9	21	0.50	1.012	8.89–2	0.51	8.96–4	3
				Rejected data				
85KAR/ABD1	(4.52–2, 0.26,–3.10–2, –5)							

TABLE 44.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	21	1.064	9.35–2	0.53	8.96–4	3
Temp. range K		A_1	A_2				Level of uncertainty
289.3–342.9		6.60712	3.61453				IV

TABLE 44.3.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.972	2.006	2.013	2.055	2.097	2.139	2.180
C_p ($J K^{-1} mol^{-1}$)	142.1	144.5	145.1	148.1	151.1	154.1	157.1

TABLE 44.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	21	1.093	9.60–2	0.55	8.95–4	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
289.3–342.9	616.00	–9.43508–2	1.00828–4	6.63790	2.20725+1		IV

Name: Propanoic acid
Formula: $C_3H_6O_2$

CAS–RN: 79–09–4
Group No.: 44–004
Molar Mass: 74.08

TABLE 44.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86LUD	N	309.1	1	nosp	not specified		C_{avg}	DSIO	*86LUD
02LOU2	N	351.7	1	nosp	not specified		C_{avg}	DSIO	*98LOU
34RAD/JUL		289.1	1	nosp	not specified		C_p	BSIO	49WEI
71KON/WAD		298.1	1	nosp	99.80	melpt	C_p	BSIO	70LKB/COM
78WOY/KAL		303.1	1	nosp	not specified		C_p	BSIO	70REC
81CAS/WIL		298.1	1	nosp	99.5	melpt	C_p	FSIT	71PIC/LED
82MAR/AND		254.8–353.1	49	nosp	99.93	melpt	C_p	BSAO	68WES/FUR
82MAR/AND		303.4–447.1	25	nosp	99.93	melpt	C_p	BSAO	68WES/FUR

*86LUD average value in temperature range 295–323 K
02LOU2 average value in temperature range 294–410 K

TABLE 44.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82MAR/AND	254.8–353.1	49	0.10#	0.485	8.94–3	0.05	–2.28–3	–8
82MAR/AND	303.4–447.1	25	0.30#	1.097	6.73–2	0.33	4.09–2	11
				Rejected data				
*86LUD	(7.11–1, 3.65, 7.11–1, 1)			02LOU2	(3.52–1, 1.69, 3.52–1, 1)			
34RAD/JUL	(1.11, 5.79, 1.11, 1)			71KON/WAD	(2.11–1, 1.16,–2.11–1, –1)			
78WOY/KAL	(4.18–2, 0.22, 4.18–2, 1)			81CAS/WIL	(7.18–2, 0.39, –7.18–2, –1)			

TABLE 44.4.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	80	74	0.776	4.12–2	0.20	1.23–2	3
C_{sat}	80	74	0.776	4.12–2	0.20	1.23–2	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
254.8–360.0	2.75487+1	–1.32009+1	4.56932	–3.93760–1	II
360.0–447.1	3.48995+1	–1.93266+1	6.27089	–5.51313–1	III
254.8–360.0	2.77987+1	–1.34556+1	4.65537	–4.03396–1	II
360.0–447.1	3.67635+1	–2.09263+1	6.73056	–5.95544–1	III

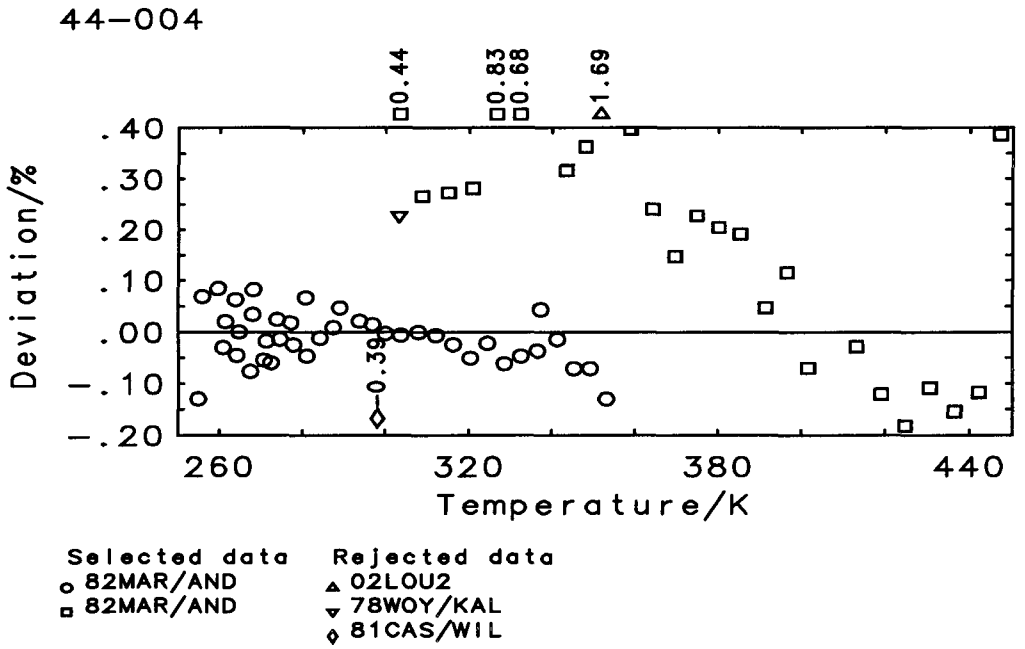
TABLE 44.4.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.930	1.960	1.971	1.994	2.030	2.062	2.069
C_p ($J K^{-1} mol^{-1}$)	143.0	145.2	146.0	147.7	150.4	152.8	153.3
c_{sat} ($J K^{-1} g^{-1}$)	1.930	1.960	1.971	1.994	2.030	2.062	2.069
C_{sat} ($J K^{-1} mol^{-1}$)	143.0	145.2	146.0	147.7	150.4	152.8	153.3
Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	2.111	2.154	2.199	2.246	2.294	2.343	2.392
C_p ($J K^{-1} mol^{-1}$)	156.4	159.6	162.9	166.4	169.9	173.5	177.2
c_{sat} ($J K^{-1} g^{-1}$)	2.111	2.154	2.199	2.246	2.294	2.343	2.392
C_{sat} ($J K^{-1} mol^{-1}$)	156.4	159.6	162.9	166.4	169.9	173.5	177.2
Temp. (K)	380	390	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.442	2.492	2.541	2.590	2.638	2.684	2.728
C_p ($J K^{-1} mol^{-1}$)	180.9	184.6	188.3	191.9	195.4	198.8	202.1
c_{sat} ($J K^{-1} g^{-1}$)	2.442	2.491	2.540	2.588	2.635	2.680	2.723
C_{sat} ($J K^{-1} mol^{-1}$)	180.9	184.5	188.2	191.7	195.2	198.5	201.7
Temp. (K)	450						
c_p ($J K^{-1} g^{-1}$)	2.770						
C_p ($J K^{-1} mol^{-1}$)	205.2						
c_{sat} ($J K^{-1} g^{-1}$)	2.763						
C_{sat} ($J K^{-1} mol^{-1}$)	204.7						

TABLE 44.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	80	74	1.175	4.52–2	0.21	–4.99–3	–29

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
254.8–447.1	612.00	1.27487+2	9.30654	5.90301	1.22972+2	1.72600+1	1.33779+2	III



Name: 2,5–Furandione
Formula: $C_4H_2O_3$

CAS–RN: 108–31–6
Group No.: 44–005
Molar Mass: 98.06

TABLE 44.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
78MAR/CIO2	N	330.0–480.0	2	nosp	not specified	C_p	DSIO	71MAR/CIO
83DEW/DEK		327.7–357.5	13	nosp	99.87 melpt	C_p	BSAO	79SCH/OFF
83DEW/OFF		335.0–355.0	5S	nosp	not specified	C_p	BDHT	69PER/COM

78MAR/CIO2 constant value calculated from temperature dependence of enthalpy by the authors

TABLE 44.5.2. Correlated heat capacities

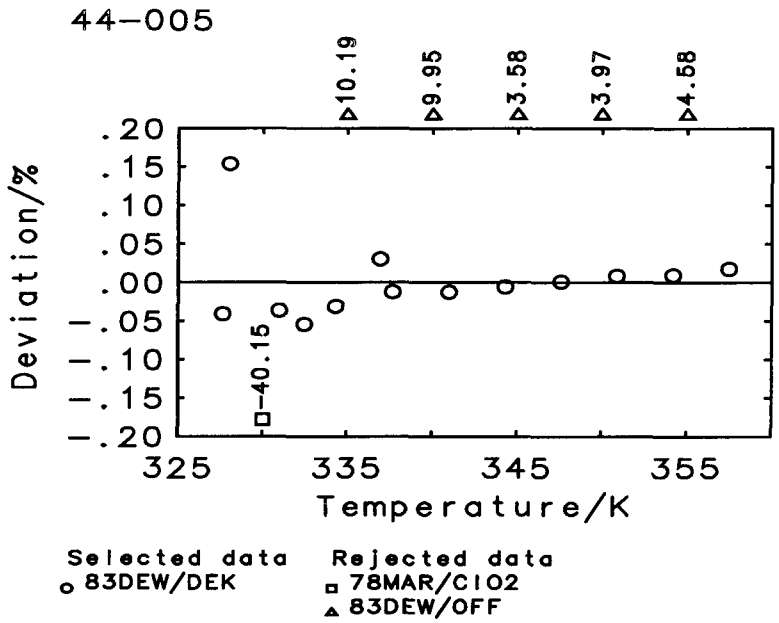
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83DEW/DEK	327.7–357.5	13	0.40#	0.124	9.40–3	0.05	9.83–6	–3
				Rejected data				
78MAR/CIO2	(5.42, 40.16, –5.42, –1)		83DEW/OFF	(1.49, 7.11, 1.34, 5)				

TABLE 44.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	13	0.135	1.02–2	0.05	9.83–6	–3
Temp. range K		A_1	A_2				Level of uncertainty
327.7–357.5		1.41168+1	1.45109				III

TABLE 44.5.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360
c_p ($J K^{-1} g^{-1}$)	1.603	1.615	1.628	1.640
C_p ($J K^{-1} mol^{-1}$)	157.2	158.4	159.6	160.8



Name: (*E*)–2–Butenoic acid
Formula: $C_4H_6O_2$

CAS–RN: 107–93–7
Group No.: 44–006
Molar Mass: 86.09

TABLE 44.6.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
25LYN	344.55	2.093	1.00	not specified		C_p	not specified	

Name: 2–Methyl–2–propenoic acid
Formula: $C_4H_6O_2$

CAS–RN: 79–41–4
Group No.: 44–007
Molar Mass: 86.09

TABLE 44.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67RAB/LEB		289.4–300.0	2S	0.50	99.92	melpt	C_p	BSAO	66NIK/LEB
85KAR/ABD2	N	288.0–350.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD2 same data in 85KAR/SAI

TABLE 44.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67RAB/LEB	289.4–300.0	2	0.50	3.999	3.84–1	2.00	2.36–1	0
85KAR/ABD2	288.0–350.4	13	0.50	0.958	9.07–2	0.48	–3.31–2	–1

TABLE 44.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	1.913	1.83–1	0.96	2.76–3	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
288.0–350.4	1.50080+1	–4.37760	1.95183	V

TABLE 44.7.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.81	1.86	1.88	1.95	2.03	2.11	2.19
C_p (J K^{-1}mol^{-1})	156	161	162	168	174	181	189

Temp. (K)	350
c_p (J K^{-1}g^{-1})	2.28
C_p (J K^{-1}mol^{-1})	196

Name: Acetic acid anhydride
Formula: $C_4H_6O_3$

CAS–RN: 108–24–7
Group No.: 44–008
Molar Mass: 102.09

TABLE 44.8.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
39PHI	303.15	1.648	nosp	not specified		C_p	BSIO	49WEI

Name: Butanoic acid
Formula: $C_4H_8O_2$

CAS–RN: 107–92–6
Group No.: 44–009
Molar Mass: 88.11

TABLE 44.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		323.6–371.5	5S	nosp	not specified		C_{avg}	DSIO	*81VON
*86LUD	N	309.6	1	nosp	not specified		C_{avg}	DSIO	*86LUD
*86SCH		321.8–350.2	8S	nosp	not specified		C_{avg}	DSIO	*86SCH
26PAR/AND		274.8–290.7	5	nosp	99.1	estim	C_p	BSIO	25PAR
71KON/WAD		298.1	1	nosp	99.8	melpt	C_p	BSIO	70LKB/COM
81CAS/WIL		298.1	1	nosp	99.5	melpt	C_p	FSIT	71PIC/LED
82MAR/AND		272.8–373.1	32	nosp	99.93	melpt	C_p	BSAO	68WES/FUR

*86LUD average value in temperature range 296–323 K

TABLE 44.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71KON/WAD	298.1	1	0.30#	0.376	2.41–2	0.11	2.41–2	1
82MAR/AND	272.8–373.1	32	0.10#	0.818	1.81–2	0.08	–5.29–5	–4
				Rejected data				
*81VON	(7.10–1, 2.96,–5.61–1, –3)			*86LUD	(4.23–1, 1.89, 4.23–1, 1)			
*86SCH	(4.56–1, 1.91, 4.23–1, 8)			26PAR/AND	(1.34–1, 0.64, 1.32–1, 5)			
81CAS/WIL	(5.64–2, 0.26,–5.64–2, –1)							

TABLE 44.9.3. Parameters of regression polynomial

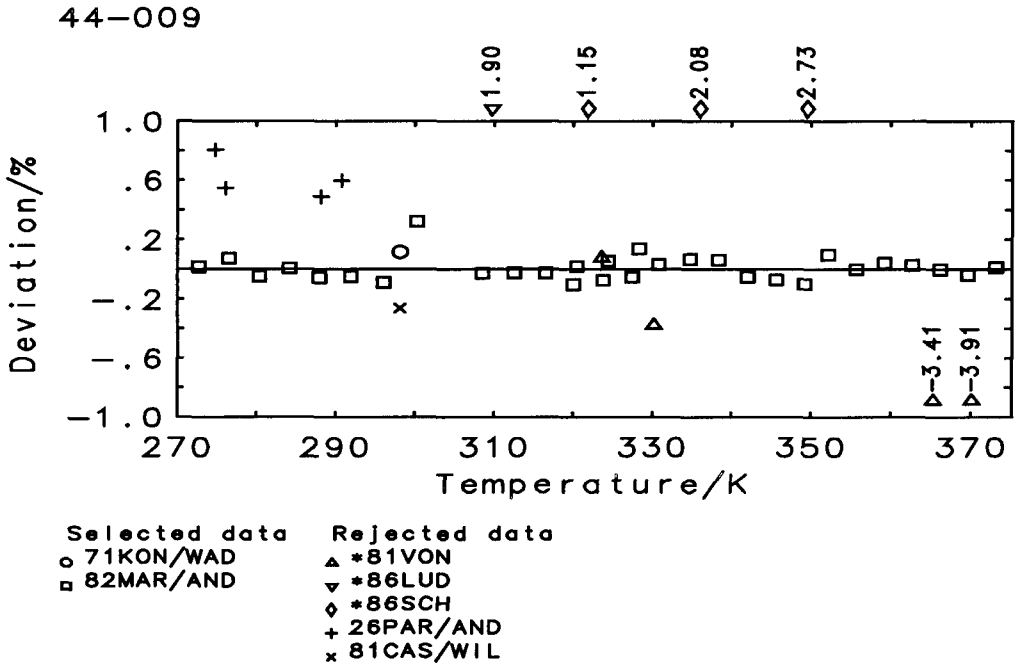
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	33	0.862	1.95–2	0.09	6.80–4	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
272.8–373.1		1.08397	1.36251+1	–3.73063	4.84463–1		II

TABLE 44.9.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	1.907	1.919	1.946	1.985	2.018	2.026	2.067
C_p ($J K^{-1}mol^{-1}$)	168.0	169.1	171.5	174.9	177.8	178.5	182.1
Temp. (K)	320	330	340	350	360	370	
c_p ($J K^{-1}g^{-1}$)	2.110	2.154	2.201	2.250	2.302	2.356	
C_p ($J K^{-1}mol^{-1}$)	185.9	189.8	193.9	198.2	202.8	207.6	

TABLE 44.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	53	33	0.874	2.00–2	0.09	–1.96–4	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
272.8–373.1	628.00	–6.85861	2.59094	9.87553	4.53894		II



Name: 2–Methylpropanoic acid
Formula: $C_4H_8O_2$

CAS–RN: 79–31–2
Group No.: 44–010
Molar Mass: 88.11

TABLE 44.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	316.0–374.3	5S	nosp	not specified		C_{avg}	DSIO	*81VON
*86SCH	322.5–350.3	7S	nosp	not specified		C_{avg}	DSIO	*86SCH
67RAB/LEB	227.2–300.0	3S	0.50	99.43	melpt	C_p	BSAO	66NIK/LEB
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

TABLE 44.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	316.0–374.3	5	2.00#	0.963	4.54–1	1.93	–5.25–2	0
67RAB/LEB	227.2–300.0	3	0.50	4.732	4.56–1	2.37	–2.81–1	–1
71KON/WAD	298.1	1	0.30#	5.536	3.45–1	1.66	3.45–1	1
				Rejected data				
*86SCH	(6.87–1, 2.93, 6.82–1, 7)							

TABLE 44.10.3. Parameters of regression polynomial

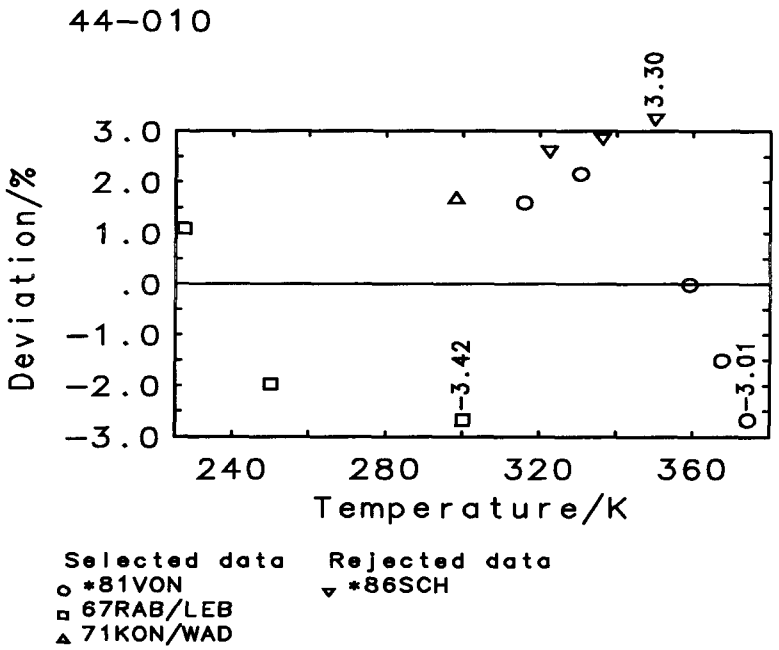
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	9	4.132	5.43–1	2.52	–8.44–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
227.2–374.3		1.43100+1	–1.03584	1.03943			V

TABLE 44.10.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	1.64	1.68	1.72	1.76	1.80	1.82	1.85
C_p ($J K^{-1} mol^{-1}$)	145	148	151	155	159	160	163
Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.89	1.93	1.94	1.99	2.04	2.10	2.15
C_p ($J K^{-1} mol^{-1}$)	167	170	171	175	180	185	190
Temp. (K)	350	360	370				
c_p ($J K^{-1} g^{-1}$)	2.21	2.27	2.33				
C_p ($J K^{-1} mol^{-1}$)	195	200	205				

TABLE 44.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	9	4.103	3.51–1	1.75	–2.86–2	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
227.2–374.3	609.00	1.26281+4	1.49555+3	–1.59428+3	1.22854+4	7.48062+2	8.37960+3	V



Name: 3–Methylbutanoic acid
Formula: $C_5H_{10}O_2$

CAS–RN: 503–74–2
Group No.: 44–011
Molar Mass: 102.13

TABLE 44.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	313.8–385.4	6S	nosp	not specified		C_{avg}	DSIO	*81VON
*86SCH	322.3–349.9	7S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 44.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	313.8–385.4	6	2.00#	0.970	4.96–1	1.94	–4.38–1	–6
*86SCH	322.3–349.9	7	2.00#	0.801	4.42–1	1.60	4.05–1	7

TABLE 44.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	13	13	0.960	5.09–1	1.92	1.59–2	1

Temp. range K	A_1	A_2	Level of uncertainty
313.8–385.4	6.74579	5.90966	V

TABLE 44.11.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c ($J K^{-1}g^{-1}$)	2.04	2.09	2.14	2.18	2.23	2.28	2.33
C ($J K^{-1}mol^{-1}$)	208	213	218	223	228	233	238
Temp. (K)	380	390					
c ($J K^{-1}g^{-1}$)	2.38	2.43					
C ($J K^{-1}mol^{-1}$)	243	248					

Name: Pentanoic acid
Formula: $C_5H_{10}O_2$

CAS–RN: 109–52–4
Group No.: 44–012
Molar Mass: 102.13

TABLE 44.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65MCD/KIL1	241.5–303.0	8	nosp	99.59	melpt	C_p	BSIO	55TAY/JOH
71KON/WAD	298.1	1	0.50	99.8	chrom	C_p	BSIO	70LKB/COM

TABLE 44.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65MCD/KIL1	241.5–303.0	8	0.30#	0.084	6.03–3	0.03	3.10–6	–1
				Rejected data				
71KON/WAD	(1.60, 6.74,–1.60, –1)							

TABLE 44.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	8	0.106	7.63–3	0.03	3.10–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
241.5–303.0		3.14668+1	–9.93338	2.63691			III

TABLE 44.12.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.857	1.882	1.910	1.943	1.954	1.980	2.022
C_p (J K^{-1}mol^{-1})	189.7	192.2	195.1	198.5	199.6	202.3	206.5
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	2.059	2.068					
C_p (J K^{-1}mol^{-1})	210.3	211.2					

TABLE 44.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	8	0.132	9.81–3	0.04	0.00	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
241.5–303.0	651.00	9.47256+1	4.92954+1	–2.84851+1	4.55060+1		III

Name: Hexanedioic acid
Formula: $C_6H_{10}O_4$

CAS-RN: 124-04-9
Group No.: 44-013
Molar Mass: 146.14

TABLE 44.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79BAB/NIS	430.0–460.0	7S	1.00	99.74	melpt	C_p	BSAO	68LEA

TABLE 44.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.830	3.47–1	0.83	4.12–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
430.0–460.0		3.68932+1	1.15259				V

TABLE 44.13.4. Recommended values of heat capacities

Temp. (K)	430	440	450	460
c_p (J K^{-1}g^{-1})	2.38	2.39	2.39	2.40
C_p (J K^{-1}mol^{-1})	348	349	350	351

Name: Hexanoic acid
Formula: $C_6H_{12}O_2$

CAS-RN: 142–62–1
Group No.: 44–014
Molar Mass: 116.16

TABLE 44.14.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON		323.3–392.2	5S	nosp	not specified	C_{avg}	DSIO	*81VON
26GAR/MAD	N	284.6	1	nosp	not specified	C_{avg}	DSIO	24GAR/RAN

26GAR/MAD average value in temperature range 270–300 K

TABLE 44.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	323.3–392.2	5	2.00#	0.153	1.02–1	0.31	5.60–4	–1

TABLE 44.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	5	0.198	1.32–1	0.40	5.60–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
323.3–392.2		1.08661+1	5.80785				VI

TABLE 44.14.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J K^{-1}g^{-1}$)	2.11	2.15	2.19	2.23	2.27	2.32	2.36
C ($J K^{-1}mol^{-1}$)	245	250	255	259	264	269	274
Temp. (K)	390						
c ($J K^{-1}g^{-1}$)	2.40						
C ($J K^{-1}mol^{-1}$)	279						

Name: Benzoic acid
Formula: $C_7H_6O_2$

CAS–RN: 65–85–0
Group No.: 44–015
Molar Mass: 122.12

TABLE 44.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	396.0–473.0	eqn	nosp	not specified	C_p	DSIO	26AND/LYN
51FUR/MCC		395.5–410.0	4S	0.30	99.997 melpt	C_p	BSAO	45SCO/MEY
67PAC		413.1	1	nosp	not specified	C_p	BDHT	79DU/COM

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 44.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
51FUR/MCC	395.5–410.0	4	0.30	0.073	6.72–3	0.02	3.78–4	1
67PAC	413.1	1	3.00#	0.157	1.48–1	0.47	–1.48–1	–1
				Rejected data				
26AND/LYN	(1.48, 4.60, 1.47, 4)							

TABLE 44.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	5	0.124	8.58–2	0.27	–2.93–2	0
Temp. range K		A_1	A_2				Level of uncertainty
395.5–413.1		–3.05261–1	7.69579				III

TABLE 44.15.4. Recommended values of heat capacities

Temp. (K)	400	410
c_p ($J K^{-1}g^{-1}$)	2.075	2.127
C_p ($J K^{-1}mol^{-1}$)	253.4	259.8

Name: Heptanoic acid
Formula: $C_7H_{14}O_2$

CAS–RN: 111–14–8
Group No.: 44–016
Molar Mass: 130.19

TABLE 44.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26GAR/MAD	N	281.0	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN1		275.0–305.0	8S	nosp	98.46	melpt	C_{sat}	BSAO	79SCH/OFF
91LAB/WES		266.4–347.8	35	nosp	98.97	melpt	C_p	BSAO	61GOO

26GAR/MAD average value in temperature range 266–296 K

TABLE 44.16.2. Correlated heat capacities

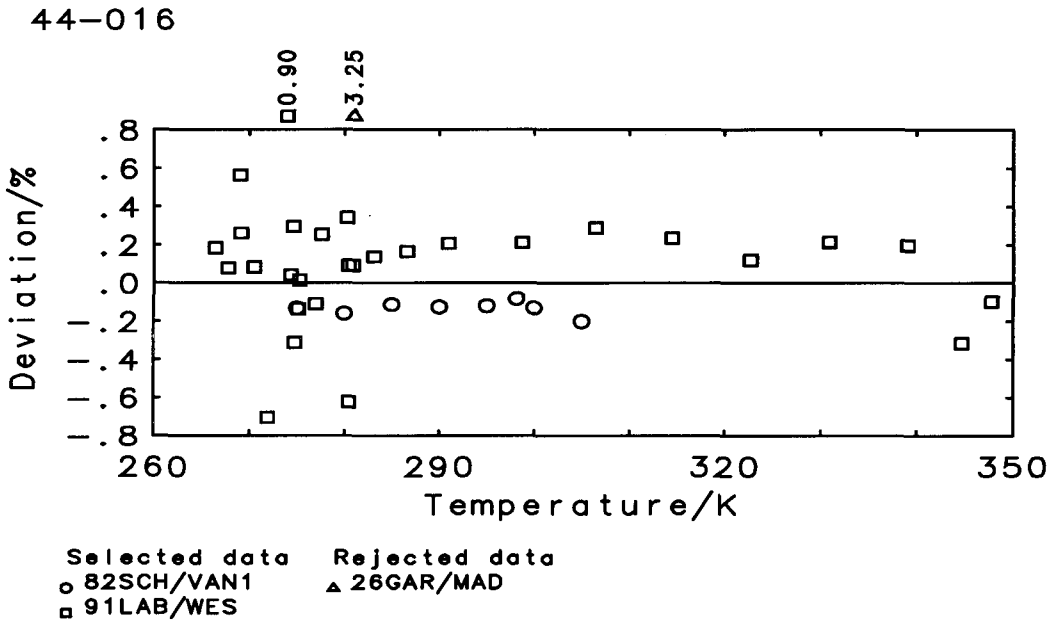
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN1	275.0–305.0	8	0.40#	0.346	4.37–2	0.14	–4.24–2	–8
91LAB/WES	266.4–347.8	34	0.50#	0.733	1.13–1	0.37	1.65–2	16
				Rejected data				
26GAR/MAD	(1.04, 3.24, 1.04, 1)							

TABLE 44.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	44	42	0.702	1.08–1	0.35	5.25–3	8
Temp. range K		A_1	A_2	A_3			Level of uncertainty
266.4–347.8		4.10211+1	–1.17989+1	2.93699			III

TABLE 44.16.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c ($J\,K^{-1}g^{-1}$)	1.953	1.961	1.980	2.012	2.041	2.047	2.086
C ($J\,K^{-1}mol^{-1}$)	254.2	255.3	257.8	261.9	265.7	266.5	271.6
Temp. (K)	320	330	340	350			
c ($J\,K^{-1}g^{-1}$)	2.129	2.176	2.226	2.280			
C ($J\,K^{-1}mol^{-1}$)	277.2	283.3	289.8	296.9			



Name: 2–Methylbenzoic acid
Formula: $C_8H_8O_2$

CAS–RN: 118–90–1
Group No.: 44–017
Molar Mass: 136.15

TABLE 44.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	377.0–473.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 44.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.000	1.91–6	0.00	–8.17–7	0
Temp. range K		A_1	A_2				Level of uncertainty
377.0–473.2		1.51896+1	5.03217				VI

TABLE 44.17.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.10	2.13	2.16	2.19	2.22	2.25	2.28
C_p (J K^{-1}mol^{-1})	285	289	294	298	302	306	310
Temp. (K)	450	460	470				
c_p (J K^{-1}g^{-1})	2.31	2.34	2.37				
C_p (J K^{-1}mol^{-1})	315	319	323				

TABLE 44.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.000	2.30–6	0.00	–1.09–6	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
377.0–473.2	772.00	3.38938–5	7.3927–12	1.51896+1	3.88484+1	VI

Name: 3–Methylbenzoic acid
Formula: $C_8H_8O_2$

CAS–RN: 99–04–7
Group No.: 44–018
Molar Mass: 136.15

TABLE 44.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	382.0–443.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 44.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	1.91–6	0.00	6.36–7	0

Temp. range K	A_1	A_2	Level of uncertainty
382.0–443.0	2.68032+1	2.81801	VI

TABLE 44.18.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440
c_p ($J\,K^{-1}g^{-1}$)	2.31	2.33	2.34	2.36	2.38	2.39
C_p ($J\,K^{-1}mol^{-1}$)	314	317	319	321	324	326

Name: 4–Methylbenzoic acid
Formula: $C_8H_8O_2$

CAS–RN: 99–94–5
Group No.: 44–019
Molar Mass: 136.15

TABLE 44.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	453.0–498.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 44.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.000	3.57–6	0.00	–4.24–7	0
Temp. range K		A_1	A_2				Level of uncertainty
453.0–497.2		–4.18284	9.46047				VI

TABLE 44.19.4. Recommended values of heat capacities

Temp. (K)	460	470	480	490	500
c_p (J K^{-1}g^{-1})	2.40	2.46	2.52	2.58	2.63
C_p (J K^{-1}mol^{-1})	327	335	343	351	359

Name: 3a,4,7,7a–Tetrahydro–1,3–isobenzofurandione
Formula: $C_8H_8O_3$

CAS–RN: 85–43–8
Group No.: 44–020
Molar Mass: 152.15

TABLE 44.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78GEI/KAR1	372.6–390.0	3S	0.35	99.1	melpt	C_p	BSAO	54STR/ICK

TABLE 44.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.640	8.61–2	0.22	4.96–4	1
Temp. range K		A_1	A_2				Level of uncertainty
372.6–390.0		–1.73835+2	5.58009+1				V

TABLE 44.20.4. Recommended values of heat capacities

Temp. (K)	380	390
c_p (J K^{-1}g^{-1})	2.09	2.39
C_p (J K^{-1}mol^{-1})	318	364

Name: Octanoic acid
Formula: $C_8H_{16}O_2$

CAS–RN: 124–07–2
Group No.: 44–021
Molar Mass: 144.21

TABLE 44.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
24GAR/RAN	N	305.1	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN2		290.0–300.0	4S	nosp	99.24	melpt	C_{sat}	BSAO	79SCH/OFF

24GAR/RAN average value in temperature range 291–319 K

TABLE 44.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN2	290.0–300.0	4	0.40#	0.093	1.32–2	0.04	1.05–5	0

TABLE 44.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	4	0.131	1.87–2	0.05	1.05–5	0

Temp. range K	A_1	A_2	Level of uncertainty
290.0–300.0	2.00301+1	5.30161	III

TABLE 44.21.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_{sat} (J $K^{-1}g^{-1}$)	2.041	2.066	2.072
C_{sat} (J $K^{-1}mol^{-1}$)	294.4	298.0	298.8

Name: 3a,4,7,7a–Tetrahydro–4–methyl–1,3–isobenzofurandione
Formula: $C_9H_{10}O_3$

CAS–RN: 5333–84–6
Group No.: 44–022
Molar Mass: 166.18

TABLE 44.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78GEI/KAR2	332.2–360.0	4S	0.30	99.6	melpt	C_p	BSAO	54STR/ICK

TABLE 44.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.192	2.03–2	0.06	2.19–5	1
Temp. range K		A_1	A_2				Level of uncertainty
332.2–360.0		−1.50884+1	1.48412+1				IV

TABLE 44.22.4. Recommended values of heat capacities

Temp. (K)	340	350	360
c_p ($J\,K^{-1}g^{-1}$)	1.770	1.844	1.918
C_p ($J\,K^{-1}mol^{-1}$)	294.1	306.4	318.8

Name: Nonanoic acid
Formula: $C_9H_{18}O_2$

CAS–RN: 112–05–0
Group No.: 44–023
Molar Mass: 158.24

TABLE 44.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24GAR/RAN	N	304.1	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
26GAR/MAD	N	295.1	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN1		290.0–305.0	5S	nosp	98.28	melpt	C_{sat}	BSAO	79SCH/OFF

24GAR/RAN average value in temperature range 291–317 K
26GAR/MAD average value in temperature range 286–305 K

TABLE 44.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN1	290.0–305.0	5	0.40#	0.166	2.61–2	0.07	3.36–5	1
				Rejected data				
24GAR/RAN	(5.76–1, 1.43, 5.76–1, 1)			26GAR/MAD	(7.58–1, 1.90, 7.58–1, 1)			

TABLE 44.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	5	0.215	3.36–2	0.09	3.36–5	1
Temp. range K		A_1	A_2				Level of uncertainty
290.0–305.0		2.15818+1	5.92067				III

TABLE 44.23.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.036	2.062	2.067	2.098
C_{sat} (J K^{-1}mol^{-1})	322.2	326.2	327.1	332.0

Name: 1*H*,3*H*–Benzo[1,2–*c*:4,5–*c*']difuran–1,3,5,7–tetrone
Formula: $C_{10}H_2O_6$

CAS–RN: 89–32–7
Group No.: 44–024
Molar Mass: 218.12

TABLE 44.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
78MAR/CIO2	N	560.0–580.0	3S	nosp	not specified	C_p	DSIO	71MAR/CIO

78MAR/CIO2 values calculated from temperature dependence of enthalpy by the authors; suspect values

Name: Decanoic acid
Formula: $C_{10}H_{20}O_2$

CAS–RN: 334–48–5
Group No.: 44–025
Molar Mass: 172.27

TABLE 44.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
24GAR/RAN	N	323.1	1	nosp	not specified	C_{avg}	DSIO	24GAR/RAN
82SCH/VAN2		310.0–345.0	8S	nosp	99.55 melpt	C_{sat}	BSAO	79SCH/OFF

24GAR/RAN average value in temperature range 308–338 K

TABLE 44.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN2	310.0–345.0	8	0.40#	0.716	1.31–1	0.29	7.67–4	0
				Rejected data				
24GAR/RAN	(1.52, 3.51,–1.52, –1)							

TABLE 44.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	8	0.826	1.51–1	0.33	7.67–4	0
Temp. range K		A_1	A_2				Level of uncertainty
310.0–345.0		1.98293+1	7.71741				III

TABLE 44.25.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	2.112	2.149	2.186	2.223	2.261
C_{sat} (J K^{-1}mol^{-1})	363.8	370.2	376.6	383.0	389.5

Name: Undecanoic acid
Formula: $C_{11}H_{22}O_2$

CAS–RN: 112–37–8
Group No.: 44–026
Molar Mass: 186.29

TABLE 44.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
24GAR/RAN	N	324.6	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN1		305.0–330.0	6S	nosp	99.38	melpt	C_{sat}	BSAO	79SCH/OFF

24GAR/RAN average value in temperature range 309–340 K

TABLE 44.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
24GAR/RAN	324.6	1	2.00#	0.017	1.70–2	0.03	–1.70–2	–1
82SCH/VAN1	305.0–330.0	6	0.40#	0.270	5.17–2	0.11	2.29–4	2

TABLE 44.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.296	5.71–2	0.12	–2.23–3	1

Temp. range K	A_1	A_2	Level of uncertainty
305.0–330.0	2.24190+1	8.08635	III

TABLE 44.26.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_{sat} (J K^{-1}g^{-1})	2.119	2.155	2.192
C_{sat} (J K^{-1}mol^{-1})	394.8	401.6	408.3

Name: Dodecanoic acid
Formula: $C_{12}H_{24}O_2$

CAS-RN: 143–07–7
Group No.: 44–027
Molar Mass: 200.32

TABLE 44.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*85STO/WIL	N	345.8	1	nosp	not specified		C_{avg}	DSIO	*85STO/WIL
24GAR/RAN	N	336.1	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN2		325.0–345.0	5S	nosp	99.6	melpt	C_{sat}	BSAO	79SCH/OFF

*85STO/WIL average value in temperature range 319–372 K
24GAR/RAN average value in temperature range 321–351 K

TABLE 44.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN2	325.0–345.0	5	0.40#	0.195	4.22–2	0.08	7.10–5	–1
				Rejected data				
24GAR/RAN	(1.90, 3.67,–1.90, –1)							

TABLE 44.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	5	0.252	5.45–2	0.10	7.10–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
325.0–345.0		1.99879+1	1.00525+1				III

TABLE 44.27.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_{sat} (J $K^{-1}g^{-1}$)	2.206	2.248	2.290
C_{sat} (J $K^{-1}mol^{-1}$)	442.0	450.4	458.7

Name: Tridecanoic acid
Formula: $C_{13}H_{26}O_2$

CAS-RN: 638–53–9
Group No.: 44–028
Molar Mass: 214.35

TABLE 44.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26GAR/MAD	N	329.1	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN1		320.0–340.0	5S	nosp	99.78	melpt	C_{sat}	BSAO	79SCH/OFF

26GAR/MAD average value in temperature range 315–343 K

TABLE 44.28.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN1	320.0–340.0	5	0.40#	0.289	6.64–2	0.12	1.50–4	–1
				Rejected data				
26GAR/MAD	(2.53, 4.26, 2.53, 1)							

TABLE 44.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	6	5	0.374	8.58–2	0.15	1.50–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
320.0–340.0		2.86204+1	8.56132				III

TABLE 44.28.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c_{sat} (J K^{-1}g^{-1})	2.173	2.206	2.239
C_{sat} (J K^{-1}mol^{-1})	465.8	472.9	480.0

Name: Tetradecanoic acid
Formula: $C_{14}H_{28}O_2$

CAS–RN: 544–63–8
Group No.: 44–029
Molar Mass: 228.38

TABLE 44.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*85STO/WIL	N	351.0	1	nosp	not specified		C_{avg}	DSIO	*85STO/WIL
26GAR/MAD	N	340.3	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN2		335.0–345.0	3S	nosp	99.64	melpt	C_{sat}	BSAO	79SCH/OFF

*85STO/WIL average value in temperature range 329–373 K
26GAR/MAD average value in temperature range 327–353 K

TABLE 44.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN2	335.0–345.0	3	0.40#	0.171	4.22–2	0.07	5.72–5	1
				Rejected data				
26GAR/MAD	(2.18, 3.65,–2.18, –1)							

TABLE 44.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	3	0.296	7.32–2	0.12	5.72–5	1
Temp. range K		A_1	A_2				Level of uncertainty
335.0–345.0		2.20814+1	1.17152+1				III

TABLE 44.29.4. Recommended values of heat capacities

Temp. (K)	340	350
c_{sat} (J K^{-1}g^{-1})	2.254	2.297
C_{sat} (J K^{-1}mol^{-1})	514.8	524.5

Name: Pentadecanoic acid
Formula: $C_{15}H_{30}O_2$

CAS-RN: 1002–84–2
Group No.: 44–030
Molar Mass: 242.40

TABLE 44.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26GAR/MAD	N	339.5	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN1		330.0–345.0	4S	nosp	99.03	melpt	C_{sat}	BSAO	79SCH/OFF

26GAR/MAD average value in temperature range 326–353 K

TABLE 44.30.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN1	330.0–345.0	4	0.40#	0.279	7.33–2	0.11	1.68–4	0
				Rejected data				
26GAR/MAD	(1.07, 1.65,–1.07, –1)							

TABLE 44.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	4	0.394	1.04–1	0.16	1.68–4	0
Temp. range K		A_1	A_2				Level of uncertainty
330.0–345.0		3.01236+1	1.04858+1				III

TABLE 44.30.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_{sat} (J K^{-1}g^{-1})	2.220	2.256	2.292
C_{sat} (J K^{-1}mol^{-1})	538.2	546.9	555.6

Name: Hexadecanoic acid
Formula: $C_{16}H_{32}O_2$

CAS-RN: 57-10-3
Group No.: 44-031
Molar Mass: 256.43

TABLE 44.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26GAR/MAD	N	349.1	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
52WAR/SIN		347.0–365.0	3S	nosp	not specified		C_p	BSAO	44BAI/TOD
67PAC		373.1	1	nosp	not specified		C_p	BDHT	79DU/COM
82SCH/VAN2		340.0–345.0	2S	nosp	99.56	melpt	C_{sat}	BSAO	79SCH/OFF

26GAR/MAD average value in temperature range 336–363 K

TABLE 44.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67PAC	373.1	1	1.00#	0.872	7.09–1	0.87	7.09–1	1
82SCH/VAN2	340.0–345.0	2	0.40#	1.850	5.18–1	0.74	–4.71–2	0
				Rejected data				
26GAR/MAD	(2.67, 3.83,–2.67, –1)		52WAR/SIN	(3.84, 4.95, 3.76, 3)				

TABLE 44.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	7	3	2.757	1.02	1.36	2.05–1	1
Temp. range K		A_1	A_2				Level of uncertainty
340.0–373.1		–4.74623+1	3.43154+1				IV

TABLE 44.31.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c (J K^{-1}g^{-1})	2.244	2.355	2.467	2.578
C (J K^{-1}mol^{-1})	575.4	604.0	632.5	661.0

Name: Heptadecanoic acid
Formula: $C_{17}H_{34}O_2$

CAS–RN: 506–12–7
Group No.: 44–032
Molar Mass: 270.46

TABLE 44.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82SCH/VAN1	340.0–350.0	3S	nosp	99.91	melpt	C_{sat}	BSAO	79SCH/OFF

TABLE 44.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	3	3	0.062	2.31–2	0.03	7.63–6	1

Temp. range K	A_1	A_2	Level of uncertainty
340.0–350.0	2.40903+1	1.45611+1	IV

TABLE 44.32.4. Recommended values of heat capacities

Temp. (K)	340	350
c_{sat} (J $K^{-1}g^{-1}$)	2.263	2.307
C_{sat} (J $K^{-1}mol^{-1}$)	611.9	624.0

Name: (Z)–9–Octadecenoic acid
Formula: $C_{18}H_{34}O_2$

CAS–RN: 112–80–1
Group No.: 44–033
Molar Mass: 282.47

TABLE 44.33.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34MEH1	290.15	2.063	1.50	not specified		C_p	BSIO	49WEI

Name: Octadecanoic acid
Formula: $C_{18}H_{36}O_2$

CAS–RN: 57–11–4
Group No.: 44–034
Molar Mass: 284.48

TABLE 44.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
50SIN/WAR	350.0	1	nosp	not specified		C_p	BSAO	44BAI/TOD
82SCH/VAN2	350.0–355.0	2S	nosp	98.87	melpt	C_{sat}	BSAO	79SCH/OFF

TABLE 44.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN2	350.0–355.0	2	0.50#	0.000	0.00	0.00	0.00	0
				Rejected data				
50SIN/WAR	(1.96, 2.42, 1.96, 1)							

TABLE 44.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	3	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
350.0–355.0		3.47081+1	1.26285+1				IV

TABLE 44.34.4. Recommended values of heat capacities

Temp. (K)	350	360
c_{sat} (J K^{-1}g^{-1})	2.306	2.343
C_{sat} (J K^{-1}mol^{-1})	656.1	666.6

Name: Nonadecanoic acid
Formula: $C_{19}H_{38}O_2$

CAS–RN: 646–30–0
Group No.: 44–035
Molar Mass: 298.51

TABLE 44.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82SCH/VAN1	345.0–355.0	3S	nosp	99.40	melpt	C_{sat}	BSAO	79SCH/OFF

TABLE 44.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	3	3	0.015	6.38–3	0.01	2.54–6	0
Temp. range K		A_1	A_2				Level of uncertainty
345.0–355.0		3.88966+1	1.26397+1				IV

TABLE 44.35.4. Recommended values of heat capacities

Temp. (K)	350	360
c_{sat} (J K^{-1}g^{-1})	2.316	2.351
C_{sat} (J K^{-1}mol^{-1})	691.2	701.7

Name: Eicosanoic acid
Formula: $C_{20}H_{40}O_2$

CAS–RN: 506–30–9
Group No.: 44–036
Molar Mass: 312.54

TABLE 44.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26GAR/MAD	N	360.6	1	nosp	not specified		C_{avg}	DSIO	24GAR/RAN
82SCH/VAN2		350.0–355.0	2S	nosp	98.46	melpt	C_{sat}	BSAO	79SCH/OFF

26GAR/MAD average value in temperature range 348–373 K

TABLE 44.36.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82SCH/VAN2	350.0–355.0	2	0.50#	0.000	0.00	0.00	0.00	0

TABLE 44.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	3	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
350.0–355.0		8.91214+1	–4.81110–1				IV

TABLE 44.36.4. Recommended values of heat capacities

Temp. (K)	350	360
c_{sat} (J $K^{-1}g^{-1}$)	2.326	2.325
C_{sat} (J $K^{-1}mol^{-1}$)	727.0	726.6

45. Esters

The ester family contains 130 compounds of which 21 were measured at one temperature only.

The large number of investigations for this group of compounds results primarily from the fact that a variety of different esters can be made available from the simple synthesis of an acid with an alcohol. Most data are, however, limited to a narrow temperature range and the overall reliability of the data are low.

The largest number of esters (46) was investigated in the last century by Schiff in an unspecified German laboratory (*86SCH, *87SCH). In most cases, these data had to be included in the correlation because for many substances, this was either the only source of data or the only one at superambient temperatures. The same holds for the 6 esters measured by von Reis (*81VON) at THA. Data reported from ICTP were obtained with a simple isoperibol calorimeter (52ERD/JAG) and more recent data were determined for 6 esters up to C_6 in an adiabatic calorimeter (87ZAB/HYN).

Several esters of interest for macromolecular (polymer) technology were investigated at CIUG (67LEB/RAB1, 69RAB/MAR, 70MAR/RAB, 83BAB/RAB, 83RAB/KHL, 85OVC/MOS, 85RAB/NOV) with an uncertainty between 0.3 to 0.5 %. SRIL reported smoothed data (79BAL/PET, 80BAL/VAS) or parameters of correlating equations (80VAS/TRE) with an error of better than 1 %. The correlating equations published by the authors from the Uzbek Academy of Sciences (85KAR/ABD1, 85KAR/ABD2) are highly doubtful (large differences are found with all other sources) and have been considered only for those substances where no other data were available.

The only data set which can be regarded as excellent in this group is that for diethyl phthalate from NBSW (67CHA/HOR). Ten esters of the decanedioic acid (sebacate acid) and five esters derived from glycerol were measured in the same laboratory (75PHI/VAL, 76PHI/MAT) using routine DSC device with 5 % reproducibility being reported. Experimental data for 6 esters of glycerol and higher fatty acids were obtained at SRNO (47CHA/SIN, 55WAR/VIC) with an estimated error of around 2 %.

The laboratory at UOTO (80SOR/TSU, 81SOR/SUG, 82SOR/YOS) studied substances related to liquid crystals and reported data for three esters.

Name: Methyl formate
Formula: $C_2H_4O_2$

CAS-RN: 107-31-3
Group No.: 45-001
Molar Mass: 60.05

TABLE 45.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34MEH2		288.1	1	1.50	not specified		C_p	BSIO	49WEI
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM
79FUC		298.1	1	0.50	99.0	chrom	C_p	BSIO	80FUC
87ZAB/HYN	N	293.3–298.8	3	0.50	96.2	anal	C_{sat}	BSAO	87ZAB/HYN

71HAL/BAL suspect value
87ZAB/HYN dominant impurity Methanol

TABLE 45.1.2. Correlated heat capacities

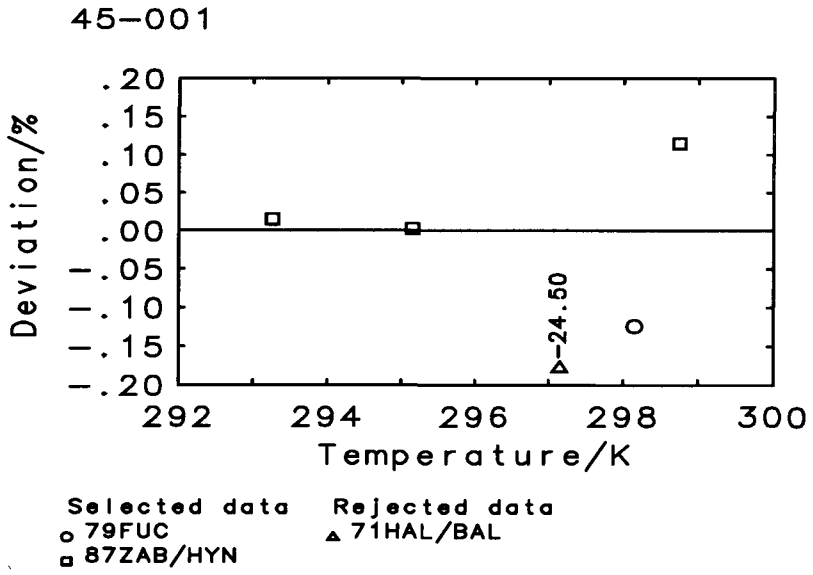
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
79FUC	298.1	1	0.50	0.253	1.82-2	0.13	-1.82-2	-1
87ZAB/HYN	293.3–298.8	3	0.50	0.132	9.53-3	0.07	6.09-3	2
				Rejected data				
71HAL/BAL	(2.81, 24.50, -2.81, -1)							

TABLE 45.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	6	4	0.241	1.74–2	0.12	2.38–5	1
Temp. range K		A_1	A_2				Level of uncertainty
293.3–298.8		-2.03895+1	1.16734+1				IV

TABLE 45.1.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c ($J K^{-1} g^{-1}$)	1.864	1.996	2.026
C ($J K^{-1} mol^{-1}$)	111.9	119.9	121.6



Name: Ethyl formate
Formula: $C_3H_6O_2$

CAS-RN: 109-94-4
Group No.: 45-002
Molar Mass: 74.08

TABLE 45.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81BER/OGI	N	304.6–306.6	2	nosp	not specified		C_{avg}	DSIO	*79BER
34KOL/UDO2	N	294.7	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
36KUR/VOS		309.0	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
79FUC		298.1	1	0.50	99.0	chrom	C_p	BSIO	80FUC

*81BER/OGI average values in temperature ranges 287–322 K and 287–326 K
34KOL/UDO2 same datum in 33KOL/UDO

TABLE 45.2.2. Correlated heat capacities

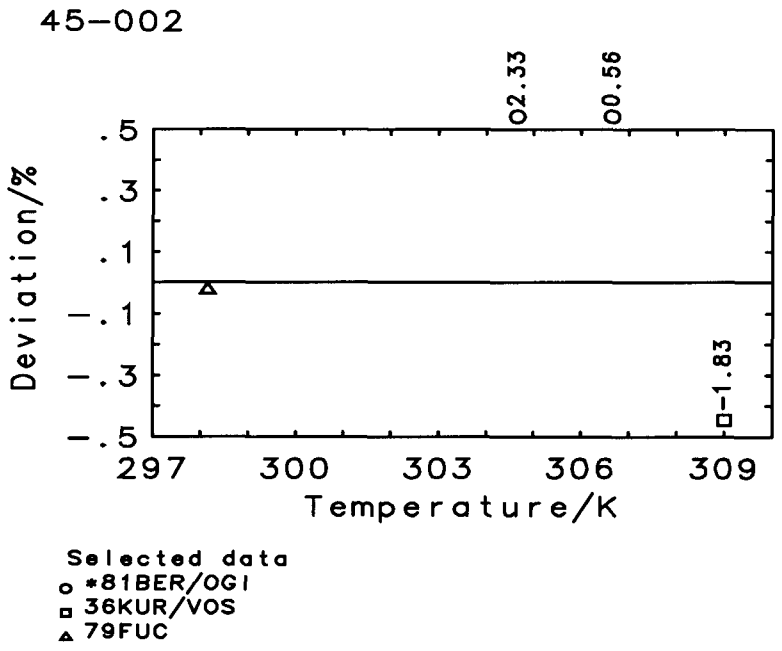
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
*81BER/OGI	304.6–306.6	2	3.00#	0.564	3.22–1	1.69	2.75–1	2
36KUR/VOS	309.0	1	3.00#	0.611	3.49–1	1.83	–3.49–1	–1
79FUC	298.1	1	0.50	0.053	4.64–3	0.03	–4.64–3	–1

TABLE 45.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	5	4	0.711	4.05–1	2.13	4.88–2	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–309.0		–3.81375+1	1.86139+1				V

TABLE 45.2.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p (J K^{-1}g^{-1})	1.99	2.20
C_p (J K^{-1}mol^{-1})	147	163



Name: Methyl acetate
Formula: $C_3H_6O_2$

CAS-RN: 79-20-9
Group No.: 45-003
Molar Mass: 74.08

TABLE 45.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26SCH		288.1	1	nosp	not specified		C_p	not specified	
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM
79FUC		298.1	1	0.50	99.0	chrom	C_p	BSIO	80FUC
85COS/PAT8		283.1–313.1	3S	nosp	99.	estim	C_p	FSIT	71PIC/LED
88PIN/BRA		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

71HAL/BAL suspect value

TABLE 45.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79FUC	298.1	1	0.80#	2.052	2.84–1	1.64	2.84–1	1
85COS/PAT8	283.1–313.1	3	1.00#	0.791	1.34–1	0.79	–1.33–1	–3
88PIN/BRA	298.1	1	1.00#	0.140	2.38–2	0.14	–2.38–2	–1
				Rejected data				
26SCH	(8.68–1, 4.97, 8.68–1, 1)			71HAL/BAL	(2.10, 14.12, –2.10, –1)			

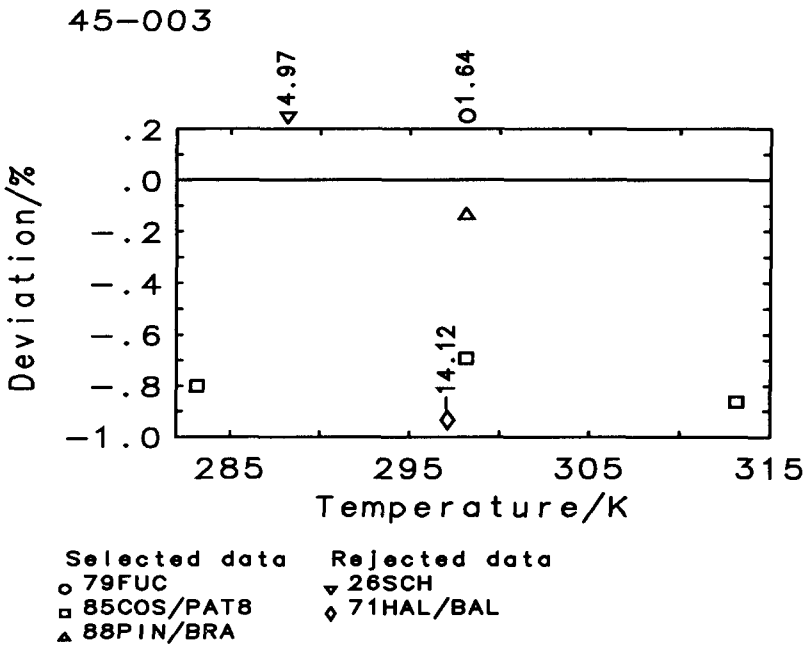
TABLE 45.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	5	1.427	2.12–1	1.24	–2.79–2	–3

Temp. range K	A_1	A_2	Level of uncertainty
283.1–313.1	4.32366	4.25937	IV

TABLE 45.3.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.824	1.872	1.911	1.919	1.967
C_p (J K^{-1}mol^{-1})	135.1	138.7	141.5	142.2	145.7



Name: Dimethyl carbonate
Formula: $C_3H_6O_3$

CAS–RN: 616–38–6
Group No.: 45–004
Molar Mass: 90.08

TABLE 45.4.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*98LOU	N	327.05	1.892	nosp	not	specified	C_{avg}	DSIO	*98LOU

*98LOU average value in temperature range 293–361 K

Name: Ethenyl acetate
Formula: $C_4H_6O_2$

CAS–RN: 108–05–4
Group No.: 45–005
Molar Mass: 86.09

TABLE 45.5.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59BEN/THO	298.15	1.966	nosp	not	specified	C_{avg}	BDHT	59BEN/THO

Name: Methyl propenoate
Formula: $C_4H_6O_2$

CAS–RN: 96–33–3
Group No.: 45–006
Molar Mass: 86.09

TABLE 45.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67LEB/RAB1		196.2–300.0	12S	0.50	99.97	melpt	C_p	BSAO	66NIK/LEB
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM
79FUC		298.1	1	0.50	99.0	chrom	C_p	BSIO	80FUC
85KAR/ABD1	N	197.0–333.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

71HAL/BAL suspect value
85KAR/ABD1 same data in 85KAR/SAI

TABLE 45.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67LEB/RAB1	196.2–300.0	12	1.00#	0.414	7.67–2	0.41	–2.85–2	–6
79FUC	298.1	1	0.80#	1.475	2.29–1	1.18	2.29–1	1
				Rejected data				
71HAL/BAL	(3.11, 19.37, –3.11, –1)			85KAR/ABD1	(1.84, 9.20, 1.83, 11)			

TABLE 45.6.3. Parameters of regression polynomial

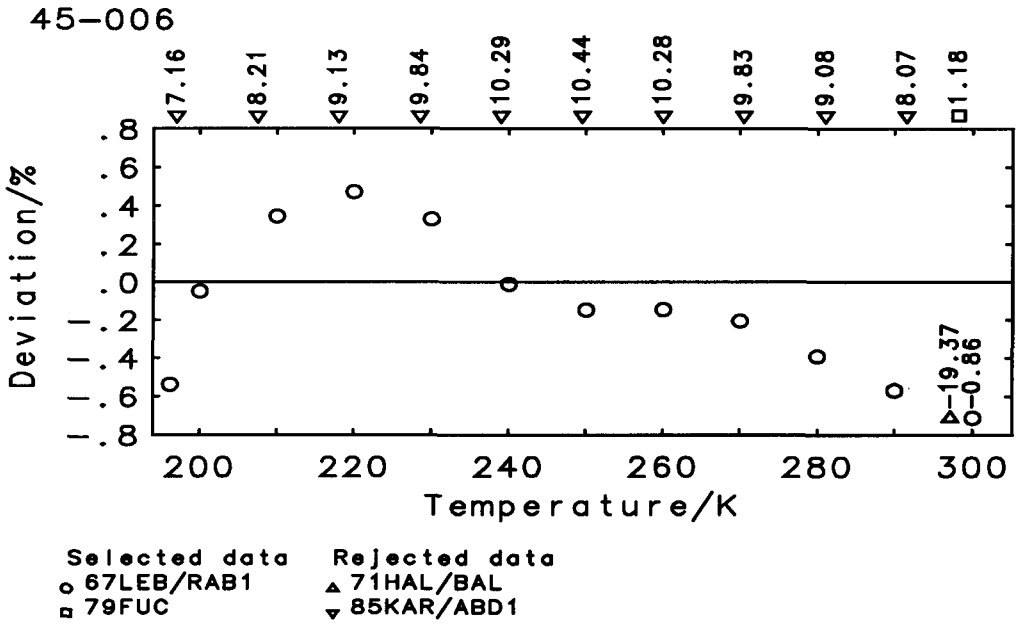
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	28	13	0.651	1.11–1	0.59	–8.66–3	–5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
196.2–300.0		2.92319+1	–1.04712+1	2.38292			IV

TABLE 45.6.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	1.721	1.714	1.712	1.715	1.722	1.733	1.750
C_p ($J K^{-1}mol^{-1}$)	148.2	147.6	147.4	147.6	148.2	149.2	150.6
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J K^{-1}g^{-1}$)	1.770	1.778	1.796	1.826	1.854	1.861	
C_p ($J K^{-1}mol^{-1}$)	152.4	153.1	154.6	157.2	159.6	160.2	

TABLE 45.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	28	13	0.609	1.00–1	0.52	6.38–3	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
196.2–300.0	536.00	1.54814+2	5.00616+1	−3.44399+1	1.19689+2		IV



Name: Ethyl acetate
Formula: $C_4H_8O_2$

CAS-RN: 141–78–6
Group No.: 45–007
Molar Mass: 88.11

TABLE 45.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	305.4–309.5	4S	nosp	not specified		C_{avg}	DSIO	*86SCH
26SCH	288.1	1	nosp	not specified		C_p	not specified	
33PAR/HUF	195.7–293.6	8	1.00	not specified		C_p	BSIO	25PAR
36KUR/VOS	309.0–309.0	2	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
45ZHD	278.2–319.1	3	nosp	not specified		C_p	BSIT	34KOL/UDO2
78ROU/PER1	283.1–313.1	3	0.30	99.8	melpt	C_p	FSIT	71PIC/LED
79FUC	298.1–298.1	2	0.50	99.0	chrom	C_p	BSIO	80FUC
85BAL/BRA	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
85COS/PAT9	283.1–313.1	3	nosp	99.5	chrom	C_p	FSIT	71PIC/LED
86JIM/ROM	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
87ZAB/HYN	293.8–340.3	11	0.50	100.0	anal	C_{sat}	BSAO	87ZAB/HYN
88PIN/BRA	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED

TABLE 45.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33PAR/HUF	195.7–293.6	8	1.00	0.520	1.03–1	0.52	9.15–2	8
78ROU/PER1	283.1–313.1	3	0.30	2.305	1.37–1	0.69	–5.25–2	1
85BAL/BRA	298.1	1	0.50#	0.416	4.23–2	0.21	–4.23–2	–1
86JIM/ROM	298.1	1	0.50#	0.132	1.35–2	0.07	–1.35–2	–1
87ZAB/HYN	293.8–340.3	11	0.50	0.995	1.04–1	0.50	3.60–2	3
88PIN/BRA	298.1	1	0.50#	0.559	5.68–2	0.28	–5.68–2	–1
				Rejected data				
*86SCH	(2.39–1, 1.14, 2.39–1, 4)			26SCH	(4.58–1, 2.23, 4.58–1, 1)			
36KUR/VOS	(1.28, 6.70,–6.07–1, 0)			45ZHD	(3.46–1, 1.69,–2.11–1, –1)			
79FUC	(2.25–1, 1.12,–2.24–1, –2)			85COS/PAT9	(2.26–1, 1.13,–2.85–2, 1)			

TABLE 45.7.3. Parameters of regression polynomial

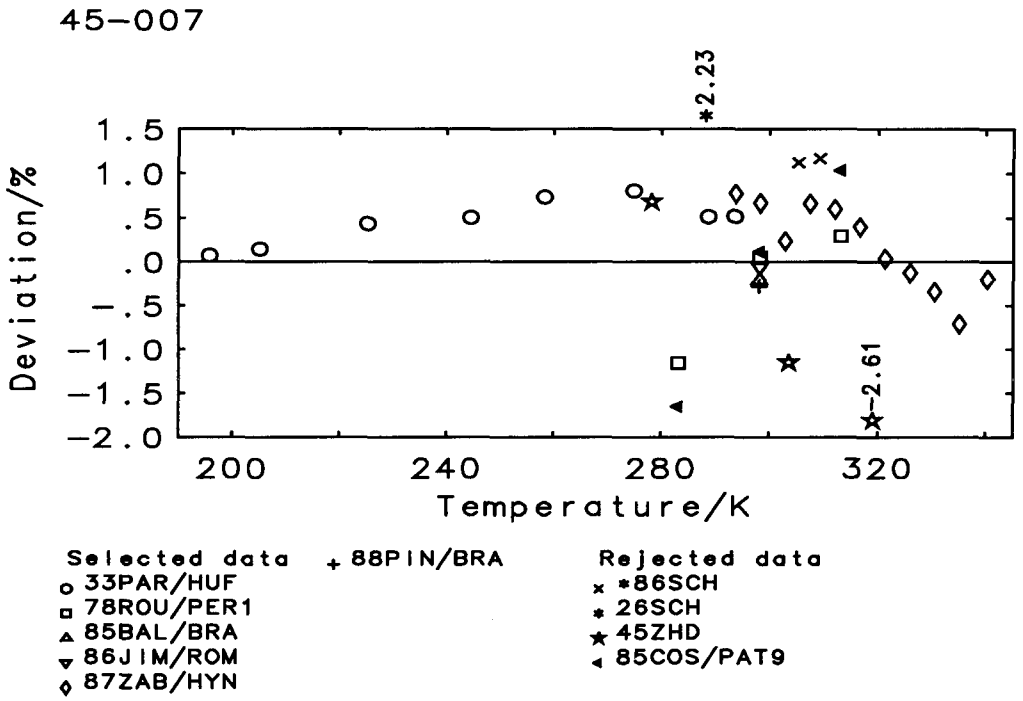
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	40	25	1.158	1.10–1	0.54	3.43–2	9
Temp. range K		A_1	A_2	A_3			Level of uncertainty
195.7–340.3		2.76771+1	–7.81959	1.80132			IV

TABLE 45.7.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c ($J K^{-1} g^{-1}$)	1.816	1.812	1.811	1.814	1.820	1.829	1.842
C ($J K^{-1} mol^{-1}$)	160.0	159.6	159.6	159.8	160.4	161.2	162.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c ($J K^{-1} g^{-1}$)	1.859	1.865	1.878	1.901	1.923	1.928	1.958
C ($J K^{-1} mol^{-1}$)	163.8	164.3	165.5	167.5	169.4	169.9	172.5
Temp. (K)	320	330	340				
c ($J K^{-1} g^{-1}$)	1.991	2.028	2.068				
C ($J K^{-1} mol^{-1}$)	175.4	178.7	182.2				

TABLE 45.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	40	24	1.489	1.08–1	0.54	–9.47–3	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
205.1–340.3	523.20	1.00584+1	5.95258	1.26661+1	4.24907		IV



Name: Methyl propanoate
Formula: $C_4H_8O_2$

CAS–RN: 554–12–1
Group No.: 45–008
Molar Mass: 88.11

TABLE 45.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*86SCH	305.8–310.3	4S	nosp	not specified	C_{avg}	DSIO	*86SCH
79FUC	298.1–298.1	2	0.50	99.0 chrom	C_p	BSIO	80FUC
84GUS/SHU	205.3–347.9	12	0.50	not specified	C_p	BSAO	54STR/ICK
85BAL/BRA	298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
86JIM/ROM	298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED
87ZAB/HYN N	295.7–341.7	9	0.50	96.5 anal	C_{sat}	BSAO	87ZAB/HYN
88PIN/BRA	298.1	1	nosp	99. anal	C_p	FSIT	71PIC/LED

87ZAB/HYN dominant impurity Methanol

TABLE 45.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79FUC	298.1	2	0.50	0.555	5.80–2	0.28	–2.08–2	0
84GUS/SHU	205.3–347.9	12	1.00#	1.199	2.64–1	1.20	1.83–1	6
86JIM/ROM	298.1	1	0.50#	1.717	1.78–1	0.86	–1.78–1	–1
87ZAB/HYN	295.7–341.7	9	0.50	0.819	8.80–2	0.41	–3.32–2	–1
				Rejected data				
*86SCH	(1.93–1, 0.92,–1.80–1, –4)			85BAL/BRA	(3.64–1, 1.77, –3.64–1, –1)			
88PIN/BRA	(3.62–1, 1.76,–3.62–1, –1)							

TABLE 45.8.3. Parameters of regression polynomial

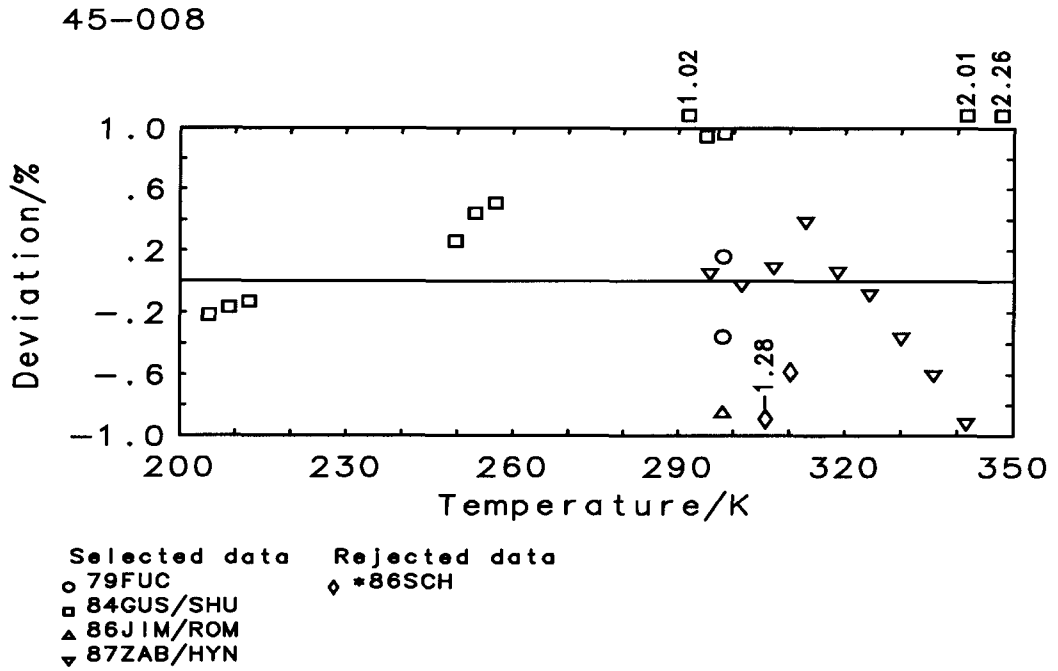
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	30	24	1.131	2.13–1	0.97	6.98–2	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
205.3–347.9		2.36633+1	−3.30980	8.05351–1			IV

TABLE 45.8.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c ($J K^{-1} g^{-1}$)	1.912	1.914	1.917	1.921	1.927	1.935	1.944
C ($J K^{-1} mol^{-1}$)	168.5	168.6	168.9	169.3	169.8	170.5	171.3
Temp. (K)	273.15	280	290	298.15	300	310	320
c ($J K^{-1} g^{-1}$)	1.947	1.954	1.966	1.977	1.980	1.995	2.012
C ($J K^{-1} mol^{-1}$)	171.5	172.2	173.3	174.2	174.5	175.8	177.3
Temp. (K)	330	340	350				
c ($J K^{-1} g^{-1}$)	2.030	2.050	2.071				
C ($J K^{-1} mol^{-1}$)	178.9	180.6	182.5				

TABLE 45.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	30	24	1.283	1.76–1	0.82	2.57–2	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
205.3–347.9	530.60	1.81568+1	7.40138	1.27591+1	1.11354+1		IV



Name: Propyl formate
Formula: $C_4H_8O_2$

CAS-RN: 110-74-7
Group No.: 45-009
Molar Mass: 88.11

TABLE 45.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	305.1–310.1	4S	nosp	not specified		C_{avg}	DSIO	*86SCH
85BAL/BRA	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
86JIM/ROM	298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED
88PIN/BRA	298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

TABLE 45.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	305.1–310.1	4	2.00#	0.133	5.57–2	0.27	–1.25–2	0
85BAL/BRA	298.1	1	0.50#	0.252	2.61–2	0.13	2.61–2	1
86JIM/ROM	298.1	1	0.50#	0.506	5.21–2	0.25	–5.21–2	–1
88PIN/BRA	298.1	1	0.50#	0.287	2.97–2	0.14	2.97–2	1

TABLE 45.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.307	5.78–2	0.28	–6.64–3	1

Temp. range K	A_1	A_2	Level of uncertainty
298.1–310.1	1.23970+1	2.77446	IV

TABLE 45.9.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	1.929	1.951	1.955	1.982
C_p ($J K^{-1} mol^{-1}$)	170.0	171.9	172.3	174.6

Name: Methyl 2-methyl-2-propenoate
Formula: $C_5H_8O_2$

CAS-RN: 80-62-6
Group No.: 45-010
Molar Mass: 100.12

TABLE 45.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52ERD/JAG		293.1–323.1	4S	1.00	not specified		C_p	BSIO	49WEI
62MEL		298.1–300.0	2S	nosp	not specified		C_p	BSAO	45SCO/MEY
67LEB/RAB1	N	225.6–300.0	9S	0.50	99.99	melpt	C_p	BSAO	66NIK/LEB
85KAR/ABD2	N	226.0–350.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA
86ZHA/BEN		298.1	1	0.30	99.9935	anal	C_p	FSIT	71PIC/LED

67LEB/RAB1 same data in 71LEB/RAB1
85KAR/ABD2 same data in 85KAR/SAI

TABLE 45.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
52ERD/JAG	293.1–323.1	4	1.00	0.774	1.87–1	0.77	–8.27–2	0
62MEL	298.1–300.0	2	0.30#	0.913	6.34–2	0.27	6.14–2	2
67LEB/RAB1	225.6–300.0	9	0.50	0.977	1.04–1	0.49	–2.85–2	1
86ZHA/BEN	298.1	1	0.30	0.064	4.43–3	0.02	4.43–3	1
				Rejected data				
85KAR/ABD2	(2.27, 9.03, 2.00, 8)							

TABLE 45.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	16	1.027	1.43–1	0.63	–2.87–2	4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
225.6–323.1		1.25478+2	–1.15192+2	4.05094+1	–4.49592		IV

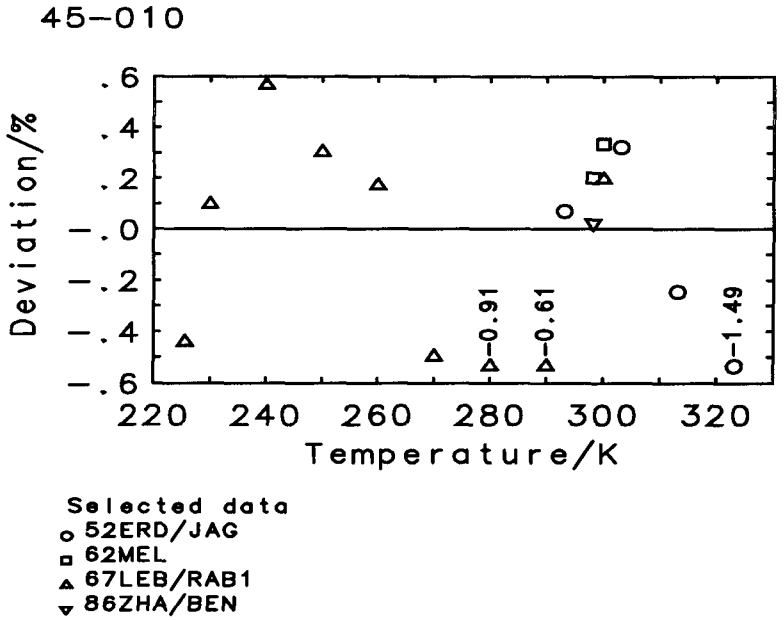
TABLE 45.10.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.672	1.678	1.697	1.728	1.767	1.781	1.814
C_p (J K^{-1}mol^{-1})	167.4	168.0	169.9	173.0	176.9	178.3	181.6
Temp. (K)	290	298.15	300	310	320		
c_p (J K^{-1}g^{-1})	1.865	1.908	1.918	1.972	2.023		
C_p (J K^{-1}mol^{-1})	186.7	191.1	192.0	197.4	202.5		

TABLE 45.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	16	0.971	1.00–1	0.48	–1.38–2	2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
225.6–323.1	565.00	4.16964+4	4.96097+3	–5.54289+3	4.19984+4	–6.29643+2	2.96228+4	IV



Name: 2-Propenyl acetate
Formula: $C_5H_8O_2$

CAS-RN: 591-87-7
Group No.: 45-011
Molar Mass: 100.12

TABLE 45.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON	324.1–337.7	4S	nosp	not specified	C_{avg}	DSIO	*81VON
*87SCH	309.0–324.0	6S	nosp	not specified	C_p	DSIO	*86SCH

TABLE 45.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	324.1–337.7	4	2.00#	0.199	9.51–2	0.40	–2.66–2	0
*87SCH	309.0–324.0	6	2.00#	0.057	2.67–2	0.11	1.83–2	4

TABLE 45.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.149	7.11–2	0.30	3.47–4	4
Temp. range K		A_1	A_2				Level of uncertainty
309.0–337.7		1.14503+1	3.82382				V

TABLE 45.11.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.94	1.97	2.00	2.03
C_p ($J K^{-1} mol^{-1}$)	194	197	200	203

Name: Butyl formate
Formula: $C_5H_{10}O_2$

CAS–RN: 592–84–7
Group No.: 45–012
Molar Mass: 102.13

TABLE 45.12.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86JIM/ROM	298.15	1.961	nosp	98.	anal	C_p	FSIT	71PIC/LED

Name: Ethyl propanoate
Formula: $C_5H_{10}O_2$

CAS–RN: 105–37–3
Group No.: 45–013
Molar Mass: 102.13

TABLE 45.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	309.6–321.7	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
86JIM/ROM	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
87ZAB/HYN	293.9–348.9	13	0.50	100.0	anal	C_{sat}	BSAO	87ZAB/HYN

TABLE 45.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86JIM/ROM	298.1	1	0.50#	1.024	1.24–1	0.51	1.24–1	1
87ZAB/HYN	293.9–348.9	13	0.50	0.351	4.29–2	0.18	–9.26–3	3
				Rejected data				
*86SCH	(3.56–1, 1.44, 3.26–1, 6)							

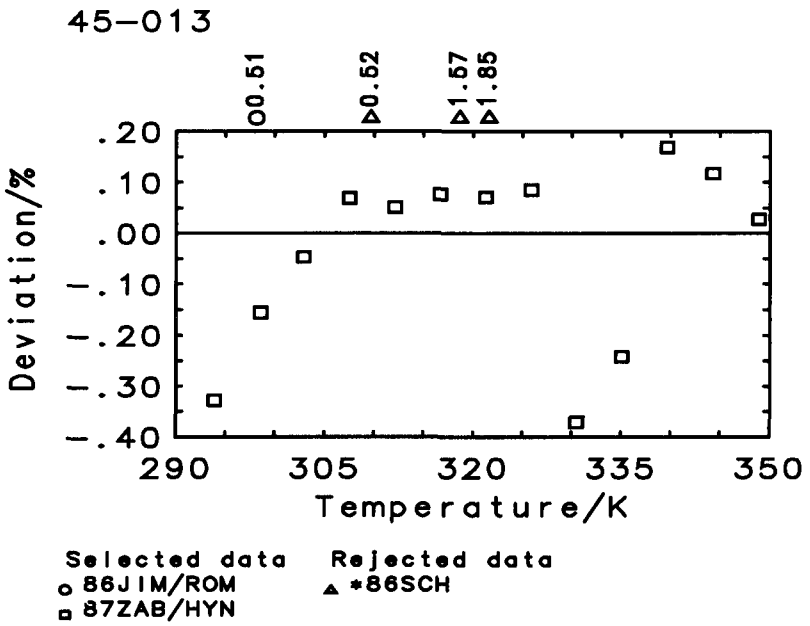
TABLE 45.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	20	14	0.491	5.97–2	0.25	2.32–4	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
293.9–348.9		5.51166+1	–2.14954+1	3.71354			III

TABLE 45.13.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c ($J K^{-1} g^{-1}$)	1.955	1.957	1.958	1.967	1.983	2.004	2.032
C ($J K^{-1} mol^{-1}$)	199.6	199.9	200.0	200.9	202.5	204.7	207.5

Temp. (K)	350
c ($J K^{-1} g^{-1}$)	2.066
C ($J K^{-1} mol^{-1}$)	211.0



Name: Methyl butanoate
Formula: $C_5H_{10}O_2$

CAS–RN: 623–42–7
Group No.: 45–014
Molar Mass: 102.13

TABLE 45.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	309.1–322.5	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
79FUC	298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC
88PIN/BRA	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED

TABLE 45.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	309.1–322.5	6	2.00#	0.185	9.00–2	0.37	–2.44–2	–1
79FUC	298.1	1	0.50	1.371	1.66–1	0.69	1.66–1	1
88PIN/BRA	298.1	1	0.50#	1.275	1.52–1	0.64	–1.52–1	–1

TABLE 45.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.786	1.29–1	0.53	–1.66–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–322.5		1.38022+1	3.41530				V

TABLE 45.14.4. Recommended values of heat capacities

Temp. (K)	300	310	320
c_p ($J K^{-1} g^{-1}$)	1.96	1.99	2.01
C_p ($J K^{-1} mol^{-1}$)	200	203	206

Name: Methyl 2–methylpropanoate
Formula: $C_5H_{10}O_2$

CAS–RN: 547–63–7
Group No.: 45–015
Molar Mass: 102.13

TABLE 45.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	308.5–322.0	5S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.003	1.43–3	0.01	–1.14–6	0
Temp. range K		A_1	A_2				Level of uncertainty
308.5–322.0		1.01848+1	4.56909				V

TABLE 45.15.4. Recommended values of heat capacities

Temp. (K)	310	320
c ($J K^{-1} g^{-1}$)	1.98	2.02
C ($J K^{-1} mol^{-1}$)	202	206

Name: 1–Methylethyl acetate
Formula: $C_5H_{10}O_2$

CAS–RN: 108–21–4
Group No.: 45–016
Molar Mass: 102.13

TABLE 45.16.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79FUC	298.15	1.925	0.50	99.0	chrom	C_p	BSIO	80FUC

Name: 2–Methylpropyl formate
Formula: $C_5H_{10}O_2$

CAS–RN: 542–55–2
Group No.: 45–017
Molar Mass: 102.13

TABLE 45.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH		310.3–318.5	5S	nosp	not specified		C_{avg}	DSIO	*86SCH
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS

36KUR/VOS average value in temperature range 290–333 K

TABLE 45.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	310.3–318.5	5	2.00#	0.003	1.33–3	0.01	–7.63–7	0
				Rejected data				
36KUR/VOS	(1.16, 4.49, 1.16, 1)							

TABLE 45.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	5	0.003	1.72–3	0.01	–7.63–7	0
Temp. range K		A_1	A_2				Level of uncertainty
310.3–318.5		4.10448	6.57416				V

TABLE 45.17.4. Recommended values of heat capacities

Temp. (K)	310	320
c ($J\,K^{-1}g^{-1}$)	1.99	2.05
C ($J\,K^{-1}mol^{-1}$)	204	209

Name: Propyl acetate
Formula: $C_5H_{10}O_2$

CAS–RN: 109–60–4
Group No.: 45–018
Molar Mass: 102.13

TABLE 45.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	324.3–337.7	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*86SCH	307.7–322.7	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
86JIM/ROM	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 45.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	324.3–337.7	4	2.00#	0.288	1.45–1	0.58	–1.36–1	–4
*86SCH	307.7–322.7	6	2.00#	0.385	1.89–1	0.77	1.85–1	6
86JIM/ROM	298.1	1	0.50#	0.287	3.38–2	0.14	–3.38–2	–1

TABLE 45.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.381	1.82–1	0.74	4.84–2	1
Temp. range K	A_1	A_2					Level of uncertainty
298.1–337.7	9.74312	4.65282					V

TABLE 45.18.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.93	1.97	2.01	2.04	2.08
C_p ($J K^{-1} mol^{-1}$)	197	201	205	209	213

Name: Diethyl carbonate
Formula: $C_5H_{10}O_3$

CAS–RN: 105–58–8
Group No.: 45–019
Molar Mass: 118.13

TABLE 45.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON		335.6–351.4	3S	nosp	not specified	C_{avg}	DSIO	*81VON
*98LOU	N	344.8	1	nosp	not specified	C_{avg}	DSIO	*98LOU
34KOL/UDO2	N	294.6	1	nosp	not specified	C_p	BSIT	34KOL/UDO2

*98LOU average value in temperature range 293–396 K
34KOL/UDO2 same datum in 33KOL/UDO

TABLE 45.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	335.6–351.4	3	2.00#	0.305	1.71–1	0.61	–3.06–3	–1
*98LOU	344.8	1	5.00#	0.043	6.07–2	0.22	–6.07–2	–1
34KOL/UDO2	294.6	1	5.00#	0.127	1.61–1	0.64	1.61–1	1

TABLE 45.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.315	1.98–1	0.72	1.83–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
294.6–351.4		7.09240	6.14229				V

TABLE 45.19.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.75	1.79	1.80	1.84	1.88	1.93	1.97
C_p (J K^{-1}mol^{-1})	207	211	212	217	222	228	233
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	2.01						
C_p (J K^{-1}mol^{-1})	238						

Name: Methyl bicyclo[1.1.0]butane–1–carboxylate
Formula: $C_6H_8O_2$

CAS–RN: 4935–01–7
Group No.: 45–020
Molar Mass: 112.13

TABLE 45.20.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71HAL/BAL	N	297.15	1.720	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: Dimethyl (Z)–2–butenedioate
Formula: $C_6H_8O_4$

CAS–RN: 624–48–6
Group No.: 45–021
Molar Mass: 144.13

TABLE 45.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30WAS1	285.5–332.2	4	2.00	not specified		C_{avg}	DSIO	30WAS1

TABLE 45.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.236	1.44–1	0.47	6.80–4	0
Temp. range K		A_1	A_2				Level of uncertainty
285.5–332.2		3.47478+1	–1.24724				VI

TABLE 45.21.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c ($J K^{-1}g^{-1}$)	1.80	1.79	1.79	1.78	1.77	1.77
C ($J K^{-1}mol^{-1}$)	259	258	258	257	256	255

Name: Ethyl cyclopropanecarboxylate
Formula: $C_6H_{10}O_2$

CAS–RN: 4606–07–9
Group No.: 45–022
Molar Mass: 114.14

TABLE 45.22.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.15	1.866	0.50	99.	chrom	C_p	BSIO	80FUC

Name: Methyl cyclobutanecarboxylate
Formula: $C_6H_{10}O_2$

CAS–RN: 765–85–5
Group No.: 45–023
Molar Mass: 114.14

TABLE 45.23.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.15	1.670	nosp	99.9	chrom	C_p	BDHT	71DU/COM

71HAL/BAL suspect value

Name: 2–Propenyl propanoate
Formula: $C_6H_{10}O_2$

CAS–RN: 2408–20–0
Group No.: 45–024
Molar Mass: 114.14

TABLE 45.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	308.4–332.5	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.039	3.15–2	0.12	4.80–5	0
Temp. range K		A_1	A_2				Level of uncertainty
308.4–332.5		1.10249+1	5.08930				V

TABLE 45.24.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J K^{-1}g^{-1}$)	1.95	1.99	2.03
C_p ($J K^{-1}mol^{-1}$)	223	227	231

Name: Diethyl ethanedioate
Formula: $C_6H_{10}O_4$

CAS–RN: 95–92–1
Group No.: 45–025
Molar Mass: 146.14

TABLE 45.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		330.6–379.9	4S	nosp	not specified		C_{avg}	DSIO	*81VON
*87SCH		319.3–348.3	6S	nosp	not specified		C_p	DSIO	*86SCH
*98LOU	N	377.5	1	nosp	not specified		C_{avg}	DSIO	*98LOU
02LOU1	N	373.6	1	nosp	not specified		C_{avg}	DSIO	*98LOU
49LEE		313.0–343.0	eqn	nosp	100	anal	C_p	BDHO	33FER/MIL

*98LOU average value in temperature range 297–458 K
02LOU1 average value in temperature range 294–453 K

TABLE 45.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	330.6–379.9	4	2.00#	1.032	6.75–1	2.06	–5.12–1	–4
*87SCH	319.3–348.3	6	2.00#	0.505	3.39–1	1.01	–4.48–2	–2
*98LOU	377.5	1	5.00#	0.226	3.94–1	1.13	3.94–1	1
02LOU1	373.6	1	5.00#	0.534	9.45–1	2.67	9.45–1	1
49LEE	313.0–343.0	7	3.00#	0.791	8.26–1	2.37	7.67–1	7

TABLE 45.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.786	7.00–1	2.04	2.31–1	3
Temp. range K		A_1	A_2				Level of uncertainty
313.0–379.9		2.82138+1	1.67891				V

TABLE 45.25.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.90	1.91	1.92	1.93	1.94	1.95	1.96
C_p (J K^{-1}mol^{-1})	278	279	281	282	283	285	286
Temp. (K)	380						
c_p (J K^{-1}g^{-1})	1.97						
C_p (J K^{-1}mol^{-1})	288						

Name: 1,2-Ethanediyl diacetate
Formula: $C_6H_{10}O_4$

CAS-RN: 111-55-7
Group No.: 45-026
Molar Mass: 146.14

TABLE 45.26.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86NIL/WAD	298.15	1.842	nosp	99.9	chrom	C_p	DDCT	71KON/SUU

Name: Butyl acetate
Formula: $C_6H_{12}O_2$

CAS-RN: 123-86-4
Group No.: 45-027
Molar Mass: 116.16

TABLE 45.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34KOL/UDO2	N	292.5	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
71HAL/BAL		298.1	1	nosp	99.0	chrom	C_p	BDHT	71DU/COM
79BAL/PET		201.0-364.3	73	nosp	99.62	melpt	C_p	BSAO	77KU/COM
80VAS/TRE		196.0-280.0	eqn	1.00	99.62	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE		280.0-370.0	eqn	1.00	99.62	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE		300.0-399.0	eqn	2.00	99.62	anal	C_{sat}	BSAO	80VAS/TRE
86JIM/ROM		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
87ZAB/HYN	N	293.8-363.8	16	0.50	98.7	anal	C_{sat}	BSAO	87ZAB/HYN

34KOL/UDO2 same datum in 33KOL/UDO
87ZAB/HYN dominant impurity Butanol

TABLE 45.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
79BAL/PET	201.0-364.3	73	1.00#	0.683	1.90-1	0.68	-1.33-1	-40
80VAS/TRE	196.0-280.0	15	1.00	0.181	4.71-2	0.18	-2.26-2	0
80VAS/TRE	280.0-369.6	15	1.00	0.924	2.61-1	0.92	-2.50-1	-15
80VAS/TRE	300.0-399.0	10	2.00	0.772	4.71-1	1.54	4.22-1	10
86JIM/ROM	298.1	1	0.50#	0.051	6.97-3	0.03	-6.97-3	-1
87ZAB/HYN	293.8-363.8	16	0.50	1.621	2.27-1	0.81	2.08-1	16
				Rejected data				
34KOL/UDO2	(2.25, 7.71, 2.25, 1)			71HAL/BAL	(3.89-1, 1.41, 3.89-1, 1)			

TABLE 45.27.3. Parameters of regression polynomial

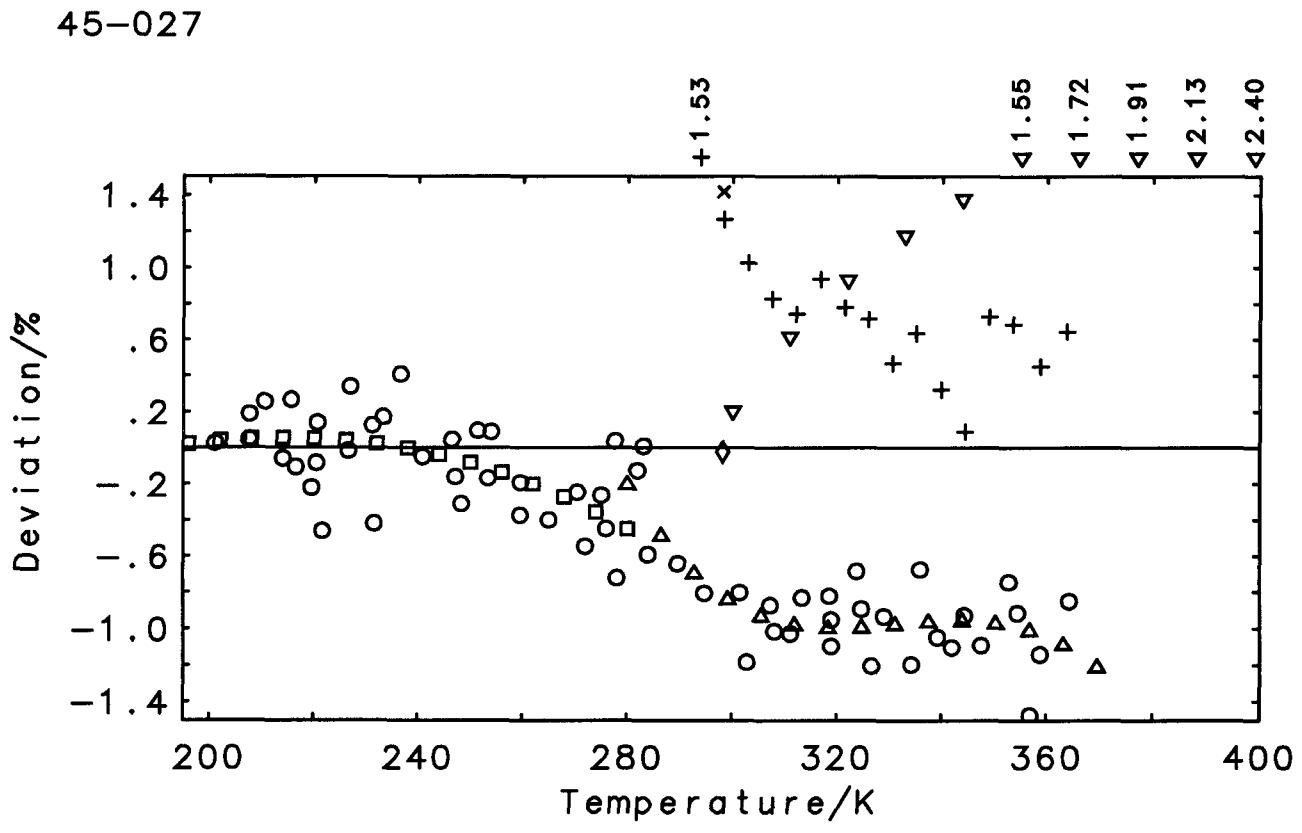
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	132	130	0.870	2.31-1	0.81	-4.82-2	-30
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
196.0-399.0	4.25214+1	-2.05062+1	7.30511	-7.25887-1			IV

TABLE 45.27.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.784	1.786	1.792	1.802	1.814	1.830	1.849
C_{sat} (J K^{-1}mol^{-1})	207.2	207.5	208.2	209.3	210.8	212.6	214.8
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.870	1.877	1.893	1.917	1.938	1.943	1.971
C_{sat} (J K^{-1}mol^{-1})	217.2	218.0	219.8	222.7	225.2	225.7	228.9
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	1.998	2.027	2.056	2.084	2.112	2.139	2.165
C_{sat} (J K^{-1}mol^{-1})	232.1	235.4	238.8	242.1	245.3	248.5	251.5
Temp. (K)	390	400					
c_{sat} (J K^{-1}g^{-1})	2.190	2.213					
C_{sat} (J K^{-1}mol^{-1})	254.4	257.1					

TABLE 45.27.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	132	130	1.053	2.15–1	0.77	6.78–3	–40
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
196.0–399.0	579.00	–7.43708–1	3.93111	1.83204+1	3.51746–2		IV



Name: 1,1–Dimethylethyl acetate
Formula: $C_6H_{12}O_2$

CAS–RN: 540–88–5
Group No.: 45–028
Molar Mass: 116.16

TABLE 45.28.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.15	1.989	0.50	99.	chrom	C_p	BSIO	80FUC

Name: Ethyl butanoate
Formula: $C_6H_{12}O_2$

CAS–RN: 105–54–4
Group No.: 45–029
Molar Mass: 116.16

TABLE 45.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH		308.5–332.4	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
34KOL/UDO2	N	297.2	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
36KUR/VOS		309.0	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
79FUC		298.1	1	0.50	99.0	chrom	C_p	BSIO	80FUC
80BAL/VAS	N	180.0–370.0	20S	nosp	not specified		C_p	not specified	

34KOL/UDO2 same datum in 33KOL/UDO
80BAL/VAS error of 0.3–1.0 % reported in 84VAS/PET

TABLE 45.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
36KUR/VOS	309.0	1	2.00#	0.009	5.12–3	0.02	5.12–3	1
79FUC	298.1	1	0.50	1.008	1.38–1	0.50	1.38–1	1
80BAL/VAS	180.0–370.0	20	1.00#	0.184	4.94–2	0.18	–2.72–2	–5
				Rejected data				
*86SCH	(2.99–1, 1.04, 2.65–1, 6)			34KOL/UDO2	(7.85–1, 2.96, –7.85–1, –1)			

TABLE 45.29.3. Parameters of regression polynomial

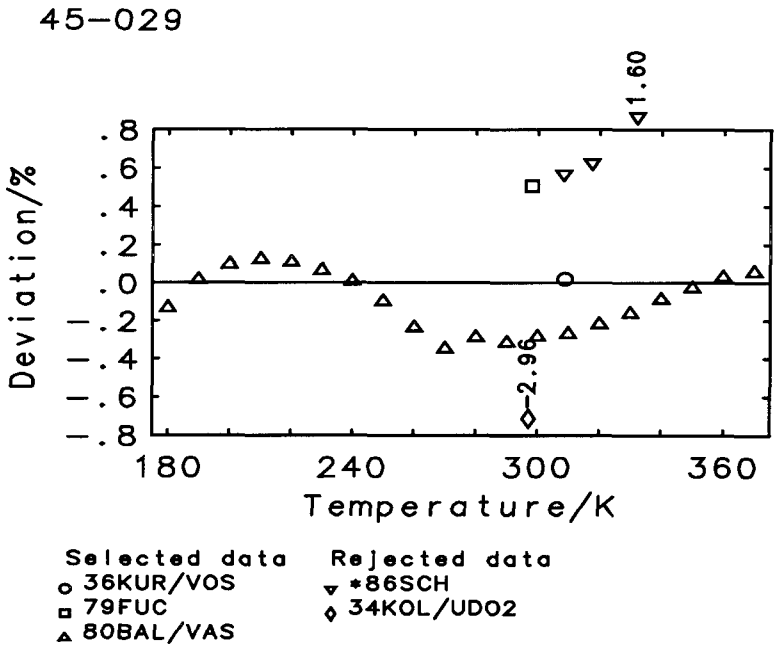
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	22	0.307	6.15–2	0.23	–1.83–2	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.0–370.0		3.99960+1	–1.66571+1	5.80076	–5.51400–1		IV

TABLE 45.29.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.832	1.826	1.823	1.825	1.829	1.837	1.847
C_p (J K^{-1}mol^{-1})	212.8	212.1	211.8	211.9	212.5	213.4	214.6
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.860	1.876	1.894	1.900	1.913	1.935	1.953
C_p (J K^{-1}mol^{-1})	216.1	217.9	220.0	220.7	222.2	224.7	226.9
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.957	1.981	2.006	2.032	2.058	2.084	2.110
C_p (J K^{-1}mol^{-1})	227.3	230.1	233.0	236.0	239.0	242.1	245.1
Temp. (K)	370						
c_p (J K^{-1}g^{-1})	2.136						
C_p (J K^{-1}mol^{-1})	248.2						

TABLE 45.29.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	20	0.551	1.24–1	0.46	–1.43–3	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.0–370.0	566.00	1.94413	4.39976	1.92619+1	2.14764–1		IV



Name: Ethyl 2–methylpropanoate
Formula: $C_6H_{12}O_2$

CAS–RN: 97–62–1
Group No.: 45–030
Molar Mass: 116.16

TABLE 45.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	308.4–327.3	5S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.002	1.35–3	0.00	3.82–7	0

Temp. range K	A_1	A_2	Level of uncertainty
308.4–327.3	1.29118+1	4.77728	V

TABLE 45.30.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	1.98	2.02	2.05
C ($J\,K^{-1}mol^{-1}$)	230	234	238

Name: Methyl 2,2–dimethylpropanoate
Formula: $C_6H_{12}O_2$

CAS–RN: 598–98–1
Group No.: 45–031
Molar Mass: 116.16

TABLE 45.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM
79FUC		298.1–298.1	2	0.50	99.0	chrom	C_p	BSIO	80FUC

71HAL/BAL suspect value

TABLE 45.31.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79FUC	298.1	2	0.50	0.000	0.00	0.00	0.00	0

TABLE 45.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.72776+1	IV

TABLE 45.31.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1} g^{-1}$)	1.952
C_p ($J K^{-1} mol^{-1}$)	226.8

Name: Methyl pentanoate
Formula: $C_6H_{12}O_2$

CAS–RN: 624–24–8
Group No.: 45–032
Molar Mass: 116.16

TABLE 45.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	308.3–332.0	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
79FUC	298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC
88PIN/BRA	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED

TABLE 45.32.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	308.3–332.0	6	2.00#	0.034	1.88–2	0.07	–2.47–3	–2
88PIN/BRA	298.1	1	0.50#	0.007	9.38–4	0.00	9.38–4	0
				Rejected data				
79FUC	(3.85–1, 1.39, 3.85–1, 1)							

TABLE 45.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.041	2.30–2	0.08	–1.98–3	–2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
298.1–332.0	3.97493+1	–1.25443+1	2.79495	V

TABLE 45.32.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.95	1.98	2.02	2.06
C_p ($J K^{-1} mol^{-1}$)	227	230	235	239

Name: 3–Methylbutyl formate
Formula: $C_6H_{12}O_2$

CAS–RN: 110–45–2
Group No.: 45–033
Molar Mass: 116.16

TABLE 45.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	309.3–333.7	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.002	1.98–3	0.01	3.18–7	1

Temp. range K	A_1	A_2	Level of uncertainty
309.3–333.7	1.04712+1	5.61140	V

TABLE 45.33.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J K^{-1} g^{-1}$)	1.99	2.03	2.07
C ($J K^{-1} mol^{-1}$)	232	236	241

Name: 2–Methylpropyl acetate
Formula: $C_6H_{12}O_2$

CAS–RN: 110–19–0
Group No.: 45–034
Molar Mass: 116.16

TABLE 45.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH		307.3–332.2	8S	nosp	not specified		C_{avg}	DSIO	*86SCH
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS

36KUR/VOS average value in temperature range 290–333 K

TABLE 45.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	307.3–332.2	8	3.00#	0.002	1.45–3	0.01	2.38–7	0
				Rejected data				
36KUR/VOS	(1.09, 3.79, 1.09, 1)							

TABLE 45.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	9	8	0.002	1.67–3	0.01	2.38–7	0
Temp. range K		A_1	A_2				Level of uncertainty
307.3–332.2		1.19983+1	5.06451				V

TABLE 45.34.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J K^{-1} g^{-1}$)	1.98	2.02	2.06
C ($J K^{-1} mol^{-1}$)	230	235	239

Name: Propyl propanoate
Formula: $C_6H_{12}O_2$

CAS–RN: 106–36–5
Group No.: 45–035
Molar Mass: 116.16

TABLE 45.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH		307.8–331.8	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
86JIM/ROM		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED
87ZAB/HYN	N	293.8–367.3	17	0.50	97.9	anal	C_{sat}	BSAO	87ZAB/HYN

87ZAB/HYN dominant impurity Propanol

TABLE 45.35.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	307.8–331.8	6	3.00#	0.139	1.18–1	0.42	–3.95–3	–2
87ZAB/HYN	293.8–367.3	17	0.50	0.475	6.81–2	0.24	3.77–4	–3
				Rejected data				
86JIM/ROM	(3.47–1, 1.27,–3.47–1, –1)							

TABLE 45.35.3. Parameters of regression polynomial

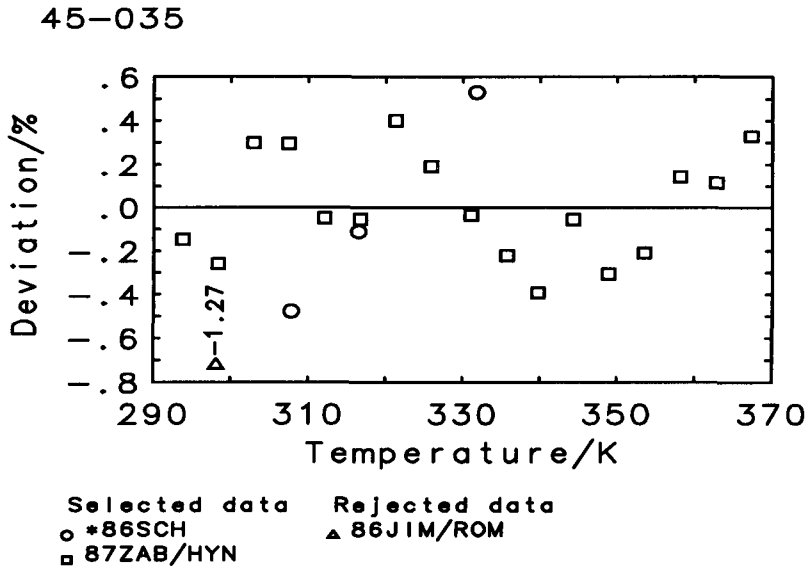
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	24	23	0.433	8.80–2	0.31	–7.50–4	–5
Temp. range K		A_1	A_2				Level of uncertainty
293.8–367.3		1.78635+1	3.26799				IV

TABLE 45.35.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c ($J K^{-1} g^{-1}$)	1.957	1.976	1.980	2.004	2.027	2.051	2.074
C ($J K^{-1} mol^{-1}$)	227.3	229.5	230.0	232.8	235.5	238.2	240.9
Temp. (K)	350	360	370				
c ($J K^{-1} g^{-1}$)	2.097	2.121	2.144				
C ($J K^{-1} mol^{-1}$)	243.6	246.3	249.1				

TABLE 45.35.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	24	23	0.454	9.47–2	0.33	–1.75–2	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
293.8–367.3	571.00	–2.56272	1.41916–1	1.94183+1	1.15694+1		IV



Name: Butyl 2-propenoate
Formula: $C_7H_{12}O_2$

CAS-RN: 141-32-2
Group No.: 45-036
Molar Mass: 128.17

TABLE 45.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
85KAR/ABD1	N	210.0–333.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD1 same data in 85KAR/SAI

TABLE 45.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.103	1.56–2	0.05	1.33–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
210.0–333.2		1.94010+1	3.81995	–6.53539–2			VI

TABLE 45.36.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.76	1.78	1.81	1.83	1.85	1.87	1.90
C_p (J K^{-1}mol^{-1})	226	229	231	234	237	240	243
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.90	1.92	1.94	1.96	1.96	1.99	2.01
C_p (J K^{-1}mol^{-1})	244	246	249	251	252	255	257
Temp. (K)	330						
c_p (J K^{-1}g^{-1})	2.03						
C_p (J K^{-1}mol^{-1})	260						

TABLE 45.36.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.106	1.59–2	0.05	1.08–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
210.0–333.2	595.00	1.34651	1.96673–2	1.95579+1	2.30469+1		VI

Name: 2–Propenyl butanoate
Formula: $C_7H_{12}O_2$

CAS–RN: 2051–78–7
Group No.: 45–037
Molar Mass: 128.17

TABLE 45.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	308.3–331.9	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.025	2.22–2	0.07	2.19–5	0
Temp. range K		A_1	A_2				Level of uncertainty
308.3–331.9		1.30473+1	5.48501				V

TABLE 45.37.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.95	1.98	2.02
C_p ($J K^{-1} mol^{-1}$)	250	254	259

Name: 2–Propenyl 2–methylpropanoate
Formula: $C_7H_{12}O_2$

CAS–RN: 15727–77–2
Group No.: 45–038
Molar Mass: 128.17

TABLE 45.38.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	308.0–332.0	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.022	2.01–2	0.07	2.04–5	0
Temp. range K		A_1	A_2				Level of uncertainty
308.0–332.0		1.26689+1	5.55127				V

TABLE 45.38.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.94	1.97	2.01
C_p ($J K^{-1} mol^{-1}$)	248	253	258

Name: Diethyl propanedioate
Formula: $C_7H_{12}O_4$

CAS–RN: 105–53–3
Group No.: 45–039
Molar Mass: 160.17

TABLE 45.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	319.4–347.8	6S	nosp	not specified		C_p	DSIO	*86SCH
33KOL/UDO	294.5	1	nosp	not specified		C_p	BSIT	34KOL/UDO2

TABLE 45.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
*87SCH	319.4–347.8	6	3.00#	0.088	9.68–2	0.26	2.44–2	2
33KOL/UDO	294.5	1	5.00#	0.228	3.91–1	1.14	–3.91–1	–1

TABLE 45.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.140	2.04–1	0.59	–3.49–2	1
Temp. range K		A_1	A_2				Level of uncertainty
294.5–347.8		1.72576+1	5.90114				V

TABLE 45.39.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.78	1.81	1.81	1.85	1.88	1.91	1.94
C_p (J K^{-1}mol^{-1})	286	290	291	296	300	305	310
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	1.97						
C_p (J K^{-1}mol^{-1})	315						

Name: Ethyl 2,2–dimethylpropanoate
Formula: $C_7H_{14}O_2$

CAS–RN: 3938–95–2
Group No.: 45–040
Molar Mass: 130.19

TABLE 45.40.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86NIL/WAD	298.15	1.930	nosp	99.9	chrom	C_p	DDCT	71KON/SUU

Name: Ethyl 3–methylbutanoate
Formula: $C_7H_{14}O_2$

CAS–RN: 108–64–5
Group No.: 45–041
Molar Mass: 130.19

TABLE 45.41.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
49LEE	313.0–343.0	eqn	nosp	99.5	estim	C_p	BDHO	33FER/MIL

TABLE 45.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	3.12–6	0.00	–1.53–6	0
Temp. range K		A_1	A_2				Level of uncertainty
313.0–343.0		1.04880+1	7.04601				V

TABLE 45.41.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340
c_p (J K^{-1}g^{-1})	2.06	2.11	2.15	2.20
C_p (J K^{-1}mol^{-1})	269	275	281	286

Name: Ethyl pentanoate
Formula: $C_7H_{14}O_2$

CAS–RN: 539–82–2
Group No.: 45–042
Molar Mass: 130.19

TABLE 45.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	307.6–332.2	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.002	2.25–3	0.01	3.18–7	0
Temp. range K		A_1	A_2				Level of uncertainty
307.6–332.2		1.33737+1	5.73033				V

TABLE 45.42.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	1.99	2.03	2.06
C ($J\,K^{-1}mol^{-1}$)	259	264	268

Name: 3–Methylbutyl acetate
Formula: $C_7H_{14}O_2$

CAS–RN: 123–92–2
Group No.: 45–043
Molar Mass: 130.19

TABLE 45.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	307.9–332.9	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.002	2.16–3	0.01	–6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
307.9–332.9		1.50861+1	5.17837				V

TABLE 45.43.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	1.99	2.02	2.05
C ($J\,K^{-1}mol^{-1}$)	259	263	268

Name: 2-Methylpropyl propanoate
Formula: $C_7H_{14}O_2$

CAS-RN: 540-42-1
Group No.: 45-044
Molar Mass: 130.19

TABLE 45.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*86SCH	309.6–333.9	6S	nosp	not specified	C_{avg}	DSIO	*86SCH

TABLE 45.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.066	6.21–2	0.20	1.54–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
309.6–333.9		1.32007+1	5.79116				V

TABLE 45.44.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J\,K^{-1}g^{-1}$)	1.99	2.03	2.06
C ($J\,K^{-1}mol^{-1}$)	259	264	269

Name: Pentyl acetate
Formula: $C_7H_{14}O_2$

CAS-RN: 628-63-7
Group No.: 45-045
Molar Mass: 130.19

TABLE 45.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
26SCH	288.1	1	nosp	not specified	C_p	not specified	
39PHI	303.3	1	nosp	not specified	C_p	BSIO	49WEI

TABLE 45.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
26SCH	288.1	1	5.00#	0.000	1.91–6	0.00	–1.91–6	0
39PHI	303.3	1	5.00#	0.000	3.82–6	0.00	–3.82–6	0

TABLE 45.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	–2.86–6	0
Temp. range K		A_1	A_2				Level of uncertainty
288.1–303.3		–3.63841+1	2.29510+1				VI

TABLE 45.45.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	1.93	2.05	2.07
C_p (J K^{-1}mol^{-1})	251	266	270

Name: Propyl butanoate
Formula: $C_7H_{14}O_2$

CAS–RN: 105–66–8
Group No.: 45–046
Molar Mass: 130.19

TABLE 45.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	317.5–346.2	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.001	1.31–3	0.00	6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
317.5–346.2		1.29334+1	5.84038				V

TABLE 45.46.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c (J K^{-1}g^{-1})	2.02	2.06	2.09	2.13
C (J K^{-1}mol^{-1})	263	268	273	277

Name: Propyl 2–methylpropanoate
Formula: $C_7H_{14}O_2$

CAS–RN: 644–49–5
Group No.: 45–047
Molar Mass: 130.19

TABLE 45.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	308.5–332.6	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.115	1.08–1	0.34	5.16–4	2
Temp. range K		A_1	A_2				Level of uncertainty
308.5–332.6		1.26973+1	5.90266				V

TABLE 45.47.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J K^{-1}g^{-1}$)	1.98	2.02	2.05
C ($J K^{-1}mol^{-1}$)	258	263	268

Name: Methyl benzoate
Formula: $C_8H_8O_2$

CAS–RN: 93–58–3
Group No.: 45–048
Molar Mass: 136.15

TABLE 45.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH		317.8–345.2	6S	nosp	not specified		C_{avg}	DSIO	*86SCH
71HAL/BAL	N	297.1	1	nosp	99.9	chrom	C_p	BDHT	71DU/COM
79FUC		298.1	1	0.50	99.0	chrom	C_p	BSIO	80FUC

71HAL/BAL suspect value

TABLE 45.48.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	317.8–345.2	6	3.00#	0.006	5.40–3	0.02	–3.68–4	0
79FUC	298.1	1	0.50	0.000	6.10–5	0.00	6.10–5	0

TABLE 45.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.008	6.61–3	0.02	–3.07–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.1–345.2		4.42857+1	–1.46601+1	2.92928			V

TABLE 45.48.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	1.63	1.65	1.67	1.70	1.73	1.76
C_p ($J K^{-1}mol^{-1}$)	222	224	228	231	235	240

Name: Di–2–propenyl ethanedioate
Formula: $C_8H_{10}O_4$

CAS–RN: 615–99–6
Group No.: 45–049
Molar Mass: 170.16

TABLE 45.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	319.0–348.0	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.016	1.89–2	0.05	1.14–5	0

Temp. range K	A_1	A_2	Level of uncertainty
319.0–348.0	2.05746+1	5.45030	V

TABLE 45.49.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.86	1.88	1.91	1.94
C_p ($J\,K^{-1}mol^{-1}$)	316	321	325	330

Name: Butyl 2–methyl–2–propenoate
Formula: $C_8H_{14}O_2$

CAS–RN: 97–88–1
Group No.: 45–050
Molar Mass: 142.20

TABLE 45.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52ERD/JAG		293.1–313.1	3S	1.00	not specified		C_p	BSIO	49WEI
85KAR/ABD2	N	197.0–350.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD2 same data in 85KAR/SAI

TABLE 45.50.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
52ERD/JAG	293.1–313.1	3	1.00	2.102	7.19–1	2.10	4.90–1	1
85KAR/ABD2	197.0–347.0	16	0.50	0.171	2.87–2	0.09	–2.15–2	–10

TABLE 45.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.899	3.03–1	0.89	5.92–2	–9
Temp. range K		A_1	A_2				Level of uncertainty
197.0–347.0		2.29001+1	3.37054				VI

TABLE 45.50.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.73	1.75	1.77	1.79	1.81	1.83	1.85
C_p (J K^{-1}mol^{-1})	246	249	252	255	258	260	263
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.87	1.88	1.89	1.91	1.93	1.93	1.95
C_p (J K^{-1}mol^{-1})	266	267	269	272	274	274	277
Temp. (K)	320	330	340	350			
c_p (J K^{-1}g^{-1})	1.97	1.99	2.01	2.03			
C_p (J K^{-1}mol^{-1})	280	283	286	288			

Name: 2–Propenyl pentanoate
Formula: $C_8H_{14}O_2$

CAS–RN: 6321–45–5
Group No.: 45–051
Molar Mass: 142.20

TABLE 45.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	318.1–347.0	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.034	3.55–2	0.10	4.26–5	0
Temp. range K		A_1	A_2				Level of uncertainty
318.1–347.0		1.49331+1	5.96381				V

TABLE 45.51.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p (J K^{-1}g^{-1})	1.99	2.02	2.06	2.09
C_p (J K^{-1}mol^{-1})	283	288	293	298

Name: Diethyl butanedioate
Formula: $C_8H_{14}O_4$

CAS–RN: 123–25–1
Group No.: 45–052
Molar Mass: 174.20

TABLE 45.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	318.1–348.7	11S	nosp	not specified	C_p	DSIO	*86SCH
34KOL/UDO2 N	292.6	1	nosp	not specified	C_p	BSIT	34KOL/UDO2
79FUC	298.1	1	0.50	99. chrom	C_p	BSIO	80FUC

34KOL/UDO2 same datum in 33KOL/UDO

TABLE 45.52.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*87SCH	318.1–348.7	11	3.00#	0.053	6.66–2	0.16	2.71–3	–1
79FUC	298.1	1	0.50	0.004	7.67–4	0.00	–7.67–4	0

TABLE 45.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	12	0.058	7.36–2	0.18	2.42–3	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.1–348.7		–1.37133+1	2.82093+1	–3.44707			V

TABLE 45.52.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.90	1.94	1.97	2.00	2.02	2.04
C_p ($J\,K^{-1}mol^{-1}$)	332	338	343	348	352	356

Name: Dipropyl ethanedioate
Formula: $C_8H_{14}O_4$

CAS–RN: 615–98–5
Group No.: 45–053
Molar Mass: 174.20

TABLE 45.53.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	319.1–347.5	6S	nosp	not specified	C_p	DSIO	*86SCH

TABLE 45.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.027	3.26–2	0.08	3.12–5	0
Temp. range K		A_1	A_2				Level of uncertainty
319.1–347.5		1.98315+1	6.15856				V

TABLE 45.53.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p (J K^{-1}g^{-1})	1.89	1.92	1.95	1.98
C_p (J K^{-1}mol^{-1})	329	334	339	344

Name: 1,2–Ethanediyl dipropanoate
Formula: $C_8H_{14}O_4$

CAS–RN: 123–80–8
Group No.: 45–054
Molar Mass: 174.20

TABLE 45.54.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86NIL/WAD	298.15	1.905	nosp	99.9	chrom	C_p	DDCT	71KON/SUU

Name: Butyl butanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 109–21–7
Group No.: 45–055
Molar Mass: 144.21

TABLE 45.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79BAL/PET	192.1–366.5	65	nosp	99.41	melpt	C_p	BSAO	77KU/COM
80VAS/TRE	182.0–280.0	eqn	1.00	99.41	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	280.0–370.0	eqn	1.00	99.41	anal	C_{sat}	BSAO	80VAS/TRE
80VAS/TRE	310.0–439.0	eqn	2.00	99.41	anal	C_{sat}	BSAO	80VAS/TRE

TABLE 45.55.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79BAL/PET	192.1–366.5	65	0.80#	0.239	6.35–2	0.19	–6.38–3	–6
80VAS/TRE	182.0–280.8	20	1.00	0.079	2.50–2	0.08	1.97–4	–2
80VAS/TRE	280.0–369.3	20	1.00	0.155	5.70–2	0.16	–9.02–3	6
80VAS/TRE	310.0–438.8	15	2.00	0.352	2.66–1	0.70	2.31–1	12

TABLE 45.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	120	120	0.231	1.10–1	0.30	2.40–2	10
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
182.0–438.8		4.19771+1	–1.28294+1	4.38557	–3.36477–1		IV

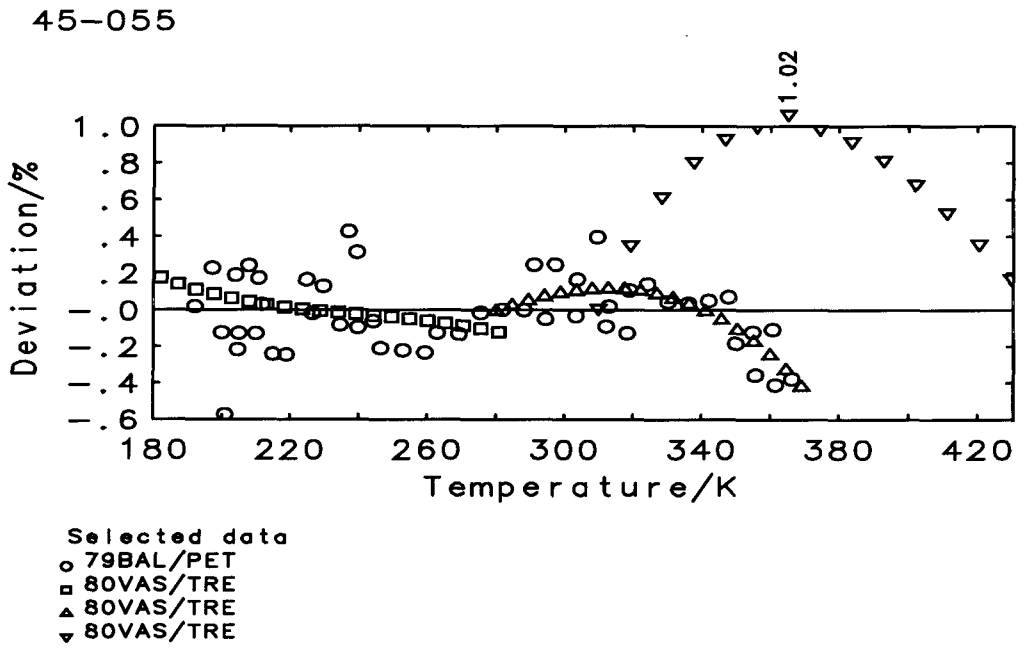
TABLE 45.55.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.795	1.797	1.802	1.810	1.820	1.833	1.848
C_{sat} (J K^{-1}mol^{-1})	258.8	259.2	259.9	261.0	262.5	264.4	266.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.865	1.884	1.891	1.906	1.928	1.948	1.953
C_{sat} (J K^{-1}mol^{-1})	269.0	271.8	272.7	274.8	278.1	281.0	281.6
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	1.979	2.007	2.036	2.066	2.097	2.129	2.162
C_{sat} (J K^{-1}mol^{-1})	285.4	289.4	293.6	297.9	302.4	307.1	311.8
Temp. (K)	380	390	400	410	420	430	440
c_{sat} (J K^{-1}g^{-1})	2.196	2.230	2.265	2.301	2.337	2.372	2.408
C_{sat} (J K^{-1}mol^{-1})	316.7	321.7	326.7	331.8	337.0	342.1	347.3

TABLE 45.55.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	120	120	0.306	1.09–1	0.30	–1.85–3	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
182.0–438.8	616.00	2.60335+2	1.99810+1	9.31734	2.64369+2	–1.27233+1	2.91081+2	IV



Name: Ethyl hexanoate
Formula: $C_8H_{16}O_2$

CAS-RN: 123-66-0
Group No.: 45-056
Molar Mass: 144.21

TABLE 45.56.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
80BAL/VAS	N	210.0–370.0	17S	1.00	not specified	C_p	not specified	

80BAL/VAS error of 0.3–1.0 % reported in 84VAS/PET

TABLE 45.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.114	3.80–2	0.11	7.00–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
210.0–370.0		4.39560+1	–1.44742+1	4.97960	–4.10669–1		IV

TABLE 45.56.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.829	1.836	1.846	1.858	1.872	1.889	1.908
C_p (J K^{-1}mol^{-1})	263.7	264.7	266.2	267.9	270.0	272.4	275.2
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.914	1.929	1.951	1.971	1.975	2.001	2.028
C_p (J K^{-1}mol^{-1})	276.1	278.1	281.4	284.2	284.9	288.6	292.4
Temp. (K)	330	340	350	360	370		
c_p (J K^{-1}g^{-1})	2.056	2.085	2.115	2.146	2.178		
C_p (J K^{-1}mol^{-1})	296.5	300.7	305.1	309.5	314.0		

TABLE 45.56.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.272	9.02–2	0.27	3.81–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
210.0–370.0	613.60	3.60159	8.07238	2.06650+1	4.01724–1		IV

Name: Hexyl acetate
Formula: $C_8H_{16}O_2$

CAS–RN: 142–92–7
Group No.: 45–057
Molar Mass: 144.21

TABLE 45.57.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80BAL/PET	N	220.0–370.0	16S	1.00	not specified		C_p	not specified	

80BAL/PET error of 0.3–1.0 % reported in 84VAS/PET

TABLE 45.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.013	4.31–3	0.01	–2.03–6	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
220.0–370.0	4.46184+1	–1.54617+1	5.35856	–4.60701–1	IV

TABLE 45.57.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.824	1.833	1.845	1.860	1.876	1.895	1.901
C_p (J K^{-1}mol^{-1})	263.0	264.4	266.1	268.2	270.6	273.3	274.2
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.915	1.938	1.957	1.961	1.987	2.013	2.041
C_p (J K^{-1}mol^{-1})	276.2	279.4	282.2	282.9	286.5	290.3	294.3
Temp. (K)	340	350	360	370			
c_p (J K^{-1}g^{-1})	2.069	2.098	2.128	2.158			
C_p (J K^{-1}mol^{-1})	298.4	302.6	306.9	311.2			

TABLE 45.57.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.211	7.19–2	0.21	2.32–4	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
220.0–370.0	623.50	7.39479–1	6.97108	2.10546+1	1.96106–2	IV

Name: Methyl heptanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 106–73–0
Group No.: 45–058
Molar Mass: 144.21

TABLE 45.58.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.1–298.1	2	0.50	99.	chrom	C_p	BSIO	80FUC

TABLE 45.58.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.198	3.40–2	0.10	3.24–5	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.42894+1	IV

TABLE 45.58.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J $K^{-1}g^{-1}$)	1.977
C_p (J $K^{-1}mol^{-1}$)	285.1

Name: 3–Methylbutyl propanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 105–68–0
Group No.: 45–059
Molar Mass: 144.21

TABLE 45.59.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH		316.3–344.5	5S	nosp	not specified		C_{avg}	DSIO	*86SCH
84GUS/SHU	N	220.4–369.7	12	0.50	not specified		C_p	BSAO	54STR/ICK

84GUS/SHU same data in 86GUS/KLI; calorimeter modified for continuous heating

TABLE 45.59.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
*86SCH	316.3–344.5	5	3.00#	0.170	1.85–1	0.51	1.17–1	1
84GUS/SHU	220.4–369.7	12	0.50	0.082	1.43–2	0.04	–1.32–3	0

TABLE 45.59.3. Parameters of regression polynomial

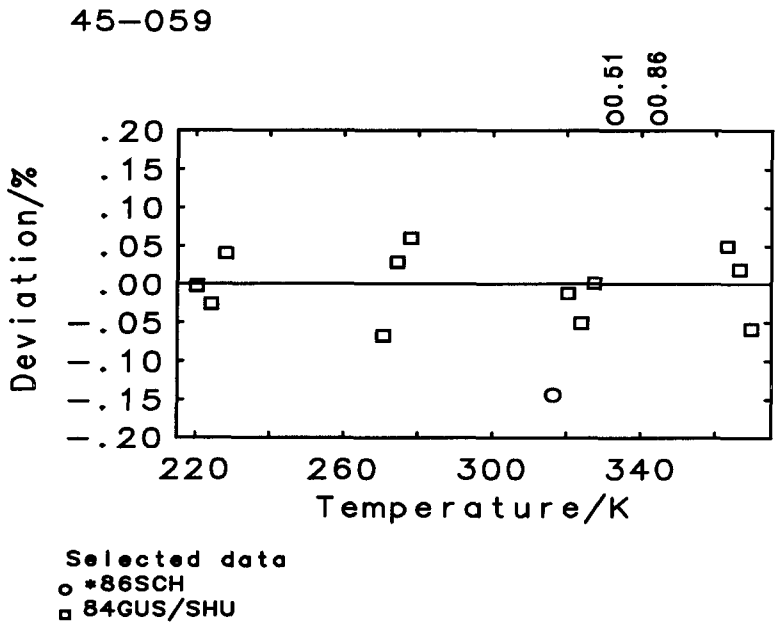
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	0.132	1.16–1	0.32	3.35–2	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
220.4–369.7		4.20223+1	–1.19545+1	3.99355	–2.88418–1		IV

TABLE 45.59.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.844	1.853	1.865	1.879	1.895	1.913	1.919
C_p (J K^{-1}mol^{-1})	265.9	267.3	269.0	271.0	273.3	275.9	276.8
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.933	1.955	1.974	1.978	2.003	2.030	2.058
C_p (J K^{-1}mol^{-1})	278.8	281.9	284.7	285.3	288.9	292.8	296.8
Temp. (K)	340	350	360	370			
c_p (J K^{-1}g^{-1})	2.087	2.118	2.150	2.182			
C_p (J K^{-1}mol^{-1})	301.0	305.4	310.0	314.7			

TABLE 45.59.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	17	1.290	2.30–1	0.70	7.58–2	–5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
220.4–369.7	611.00	–5.55294	3.27501	2.30328+1	2.35382		IV



Name: 2–Methylpropyl butanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 539–90–2
Group No.: 45–060
Molar Mass: 144.21

TABLE 45.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	318.3–345.5	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.60.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
$C_{.}$	6	6	0.003	2.72–3	0.01	6.36–7	–1

Temp. range K	A_1	A_2	Level of uncertainty
318.3–345.5	1.35078+1	6.71056	V

TABLE 45.60.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	2.02	2.06	2.09	2.13
C ($J\,K^{-1}mol^{-1}$)	291	296	302	308

Name: 2–Methylpropyl 2–methylpropanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 97–85–8
Group No.: 45–061
Molar Mass: 144.21

TABLE 45.61.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	318.2–345.8	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.003	2.73–3	0.01	1.27–6	–1

Temp. range K	A_1	A_2	Level of uncertainty
318.2–345.8	1.29259+1	6.86649	V

TABLE 45.61.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J\,K^{-1}g^{-1}$)	2.01	2.05	2.09	2.13
C ($J\,K^{-1}mol^{-1}$)	290	296	302	307

Name: Pentyl propanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 624–54–4
Group No.: 45–062
Molar Mass: 144.21

TABLE 45.62.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
84GUS/SHU	N	221.6–372.4	11	0.50	not specified	C_p	BSAO	54STR/ICK

84GUS/SHU same data in 83GUS/KLI; calorimeter modified for continuous heating

TABLE 45.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	10	0.160	2.34–2	0.08	2.10–5	–1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
221.6–372.4	2.01968+1	5.98644	–1.93274	3.24170–1	IV

TABLE 45.62.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.583	1.596	1.609	1.623	1.637	1.652	1.657
C_p (J K^{-1}mol^{-1})	228.4	230.2	232.1	234.0	236.1	238.2	238.9
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.667	1.684	1.698	1.702	1.720	1.740	1.762
C_p (J K^{-1}mol^{-1})	240.5	242.9	244.9	245.4	248.1	251.0	254.0
Temp. (K)	340	350	360	370			
c_p (J K^{-1}g^{-1})	1.784	1.809	1.835	1.863			
C_p (J K^{-1}mol^{-1})	257.3	260.8	264.6	268.6			

TABLE 45.62.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	10	0.153	2.24–2	0.08	2.31–5	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
221.6–372.4	617.80	–1.25114	4.49153	1.99124+1	8.71276–2	IV

Name: Propyl pentanoate
Formula: $C_8H_{16}O_2$

CAS–RN: 141–06–0
Group No.: 45–063
Molar Mass: 144.21

TABLE 45.63.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*86SCH	318.0–345.8	5S	nosp	not specified	C_{avg}	DSIO	*86SCH

TABLE 45.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.002	1.92–3	0.01	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
318.0–345.8		1.52776+1	6.16874				V

TABLE 45.63.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J K^{-1} g^{-1}$)	2.02	2.05	2.09	2.13
C ($J K^{-1} mol^{-1}$)	291	296	301	307

Name: Ethyl benzoate
Formula: $C_9H_{10}O_2$

CAS–RN: 93–89–0
Group No.: 45–064
Molar Mass: 150.18

TABLE 45.64.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH		318.4–345.6	5S	nosp	not specified		C_{avg}	DSIO	*86SCH
34KOL/UDO2	N	292.7	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
36KUR/VOS	N	311.6	1	nosp	not specified		C_{avg}	DSIO	36KUR/VOS
79FUC		298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC

34KOL/UDO2 same datum in 33KOL/UDO
36KUR/VOS average value in temperature range 290–333 K

TABLE 45.64.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*86SCH	318.4–345.6	5	3.00#	0.022	2.10–2	0.07	–7.97–5	–1
34KOL/UDO2	292.7	1	3.00#	0.172	1.50–1	0.52	–1.50–1	–1
79FUC	298.1	1	0.50	0.029	4.22–3	0.01	4.22–3	1
				Rejected data				
36KUR/VOS	(3.62, 10.63, 3.62, 1)							

TABLE 45.64.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	7	0.081	7.04–2	0.24	–2.09–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
292.7–345.6		1.17282+1	5.98841				V

TABLE 45.64.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.61	1.64	1.64	1.68	1.71	1.74	1.78
C_p ($J K^{-1} mol^{-1}$)	242	246	247	252	257	262	267

Temp. (K)	350
c_p ($J K^{-1} g^{-1}$)	1.81
C_p ($J K^{-1} mol^{-1}$)	272

Name: Phenylmethyl acetate
Formula: $C_9H_{10}O_2$

CAS–RN: 140–11–4
Group No.: 45–065
Molar Mass: 150.18

TABLE 45.65.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
34KOL/UDO2	N	292.7	1	nosp	not specified	C_p	BSIT	34KOL/UDO2
39PHI	N	305.9	1	nosp	not specified	C_p	BSIO	49WEI
79FUC	N	298.1	1	0.50	not specified	C_p	BSIO	80FUC

34KOL/UDO2 same datum in 33KOL/UDO
39PHI suspect value
79FUC erroneous C_p value in article corrected according to the author's communication

TABLE 45.65.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79FUC	298.1	1	0.50	0.000	0.00	0.00	0.00	0

TABLE 45.65.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.98755+1	V

TABLE 45.65.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1} g^{-1}$)	1.65
C_p ($J K^{-1} mol^{-1}$)	248

Name: 1,2,3–Propanetriol triacetate
Formula: $C_9H_{14}O_6$

CAS–RN: 102–76–1
Group No.: 45–066
Molar Mass: 218.21

TABLE 45.66.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC
83RAB/KHL	275.1–320.0	3S	0.30	99.4	melpt	C_p	BSAO	76LEB/LIT
86NIL/WAD	298.1	1	nosp	99.9	chrom	C_p	DDCT	71KON/SUU

TABLE 45.66.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83RAB/KHL	275.1–320.0	3	0.30	0.997	1.38–1	0.30	–1.38–1	–3
86NIL/WAD	298.1	1	0.30#	3.013	4.23–1	0.90	4.23–1	1
				Rejected data				
79FUC	(1.99, 4.11, 1.99, 1)							

TABLE 45.66.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	4	2.455	3.44–1	0.74	2.51–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
275.1–320.0		3.63641+1	3.35356				IV

TABLE 45.66.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_p ($J\,K^{-1}g^{-1}$)	1.743	1.756	1.767	1.769	1.782	1.795
C_p ($J\,K^{-1}mol^{-1}$)	380.4	383.2	385.5	386.0	388.8	391.6

Name: Ethyl cyclohexanecarboxylate
Formula: $C_9H_{16}O_2$

CAS–RN: 3289–28–9
Group No.: 45–067
Molar Mass: 156.22

TABLE 45.67.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.15	1.738	0.50	99.	chrom	C_p	BSIO	80FUC

Name: Dipropyl propanedioate
Formula: $C_9H_{16}O_4$

CAS–RN: 1117–19–7
Group No.: 45–068
Molar Mass: 188.22

TABLE 45.68.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	319.8–348.3	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.68.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.049	6.43–2	0.15	1.18–4	0
Temp. range K		A_1	A_2				Level of uncertainty
319.8–348.3		2.20334+1	6.51217				V

TABLE 45.68.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.89	1.92	1.95	1.98
C_p ($J\,K^{-1}mol^{-1}$)	356	362	367	373

Name: Butyl pentanoate
Formula: $C_9H_{18}O_2$

CAS–RN: 591–68–4
Group No.: 45–069
Molar Mass: 158.24

TABLE 45.69.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80BAL/PET	N	190.0–370.0	19S	1.00	not specified		C_p	not specified	

80BAL/PET error of 0.3–1.0 % reported in 84VAS/PET

TABLE 45.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.058	2.11–2	0.06	1.57–5	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
190.0–370.0		5.43883+1	–2.35336+1	8.30101	–7.81361–1		IV

TABLE 45.69.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1}g^{-1}$)	1.801	1.801	1.804	1.811	1.822	1.835	1.851
C_p ($J K^{-1}mol^{-1}$)	285.0	285.0	285.5	286.6	288.2	290.3	292.9
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.870	1.891	1.898	1.914	1.939	1.960	1.965
C_p ($J K^{-1}mol^{-1}$)	295.9	299.2	300.3	302.8	306.8	310.2	311.0
Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	1.993	2.022	2.052	2.082	2.113	2.143	2.174
C_p ($J K^{-1}mol^{-1}$)	315.4	319.9	324.6	329.4	334.3	339.2	344.0

TABLE 45.69.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.146	5.32–2	0.15	1.63–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
190.0–370.0	632.00	1.50827+3	1.59576+2	–1.32802+2	1.44449+3	1.61750+2	1.07746+3	IV

Name: Methyl octanoate
Formula: $C_9H_{18}O_2$

CAS–RN: 111–11–5
Group No.: 45–070
Molar Mass: 158.24

TABLE 45.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88PIN/BRA	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
91DES/PAT	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 45.70.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88PIN/BRA	298.1	1	0.50#	0.399	7.55–2	0.20	–7.55–2	–1
91DES/PAT	298.1	1	0.50#	0.401	7.61–2	0.20	7.61–2	1

TABLE 45.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.566	1.07–1	0.28	3.01–4	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		3.78684+1					IV

TABLE 45.70.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J K^{-1} g^{-1}$)	1.990
C_p ($J K^{-1} mol^{-1}$)	314.9

Name: 3–Methylbutyl butanoate
Formula: $C_9H_{18}O_2$

CAS–RN: 106–27–4
Group No.: 45–071
Molar Mass: 158.24

TABLE 45.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	317.9–342.9	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.001	1.63–3	0.00	–6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
317.9–342.9		1.49731+1	7.34680				V

TABLE 45.71.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J K^{-1} g^{-1}$)	2.02	2.06	2.10
C ($J K^{-1} mol^{-1}$)	320	326	332

Name: 3–Methylbutyl 2–methylpropanoate
Formula: $C_9H_{18}O_2$

CAS–RN: 2050–01–3
Group No.: 45–072
Molar Mass: 158.24

TABLE 45.72.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	317.0–345.9	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.72.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.002	2.22–3	0.01	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
317.0–345.9		1.61678+1	6.99202				V

TABLE 45.72.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J K^{-1} g^{-1}$)	2.03	2.06	2.10	2.14
C ($J K^{-1} mol^{-1}$)	320	326	332	338

Name: 2–Methylpropyl pentanoate
Formula: $C_9H_{18}O_2$

CAS–RN: 10588–10–0
Group No.: 45–073
Molar Mass: 158.24

TABLE 45.73.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*86SCH	317.7–347.3	6S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.015	1.83–2	0.05	5.72–6	–2
Temp. range K		A_1	A_2				Level of uncertainty
317.7–347.3		1.64667+1	6.90648				V

TABLE 45.73.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J K^{-1} g^{-1}$)	2.03	2.06	2.10	2.14
C ($J K^{-1} mol^{-1}$)	321	326	332	338

Name: Pentyl butanoate
Formula: $C_9H_{18}O_2$

CAS–RN: 540–18–1
Group No.: 45–074
Molar Mass: 158.24

TABLE 45.74.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80BAL/VAS	N	200.0–370.0	18S	1.00	not specified		C_p	not specified	

80BAL/VAS error of 0.3–1.0 % reported in 84VAS/PET

TABLE 45.74.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.084	3.10–2	0.08	3.92–5	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.0–370.0		5.09776+1	–1.95946+1	6.92887	–6.32204–1		IV

TABLE 45.74.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.810	1.814	1.822	1.832	1.845	1.861	1.879
C_p (J K^{-1}mol^{-1})	286.4	287.1	288.3	289.9	292.0	294.5	297.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.899	1.906	1.921	1.944	1.965	1.970	1.996
C_p (J K^{-1}mol^{-1})	300.5	301.5	304.0	307.7	310.9	311.7	315.8
Temp. (K)	320	330	340	350	360	370	
c_p (J K^{-1}g^{-1})	2.023	2.052	2.081	2.111	2.141	2.171	
C_p (J K^{-1}mol^{-1})	320.2	324.7	329.3	334.0	338.7	343.5	

TABLE 45.74.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.363	1.36–1	0.36	7.74–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.0–370.0	629.00	6.39911	1.06898+1	2.06797+1	9.57660–1		IV

Name: 2–Propenyl benzoate
Formula: $C_{10}H_{10}O_2$

CAS–RN: 583–04–0
Group No.: 45–075
Molar Mass: 162.19

TABLE 45.75.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	319.0–348.1	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.75.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.008	7.94–3	0.02	1.91–6	0
Temp. range K		A_1	A_2				Level of uncertainty
319.0–348.1		1.42469+1	5.97436				V

TABLE 45.75.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p (J K^{-1}g^{-1})	1.71	1.74	1.77	1.80
C_p (J K^{-1}mol^{-1})	277	282	287	292

Name: Dimethyl 1,2-benzenedicarboxylate
Formula: $C_{10}H_{10}O_4$

CAS-RN: 131-11-3
Group No.: 45-076
Molar Mass: 194.19

TABLE 45.76.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78MIL		274.0–370.0	eqn	1.00	99.	chrom	C_p	BDHT	69PER/COM
86RAB/NOV	N	274.2–360.0	11S	0.50	not specified		C_p	BDAO	51POP/GAL

86RAB/NOV some data in 69RAB/MAR and 70MAR/RAB; adiabatic calorimeter 56POP/KOL used below 300 K

TABLE 45.76.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86RAB/NOV	274.2–360.0	11	0.50	0.121	2.26–2	0.06	2.46–5	–5
				Rejected data				
78MIL	(7.43–1, 1.96, 7.42–1, 10)							

TABLE 45.76.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	11	0.134	2.50–2	0.07	2.46–5	–5

Temp. range K	A_1	A_2	Level of uncertainty
274.2–360.0	2.41842+1	4.10572	IV

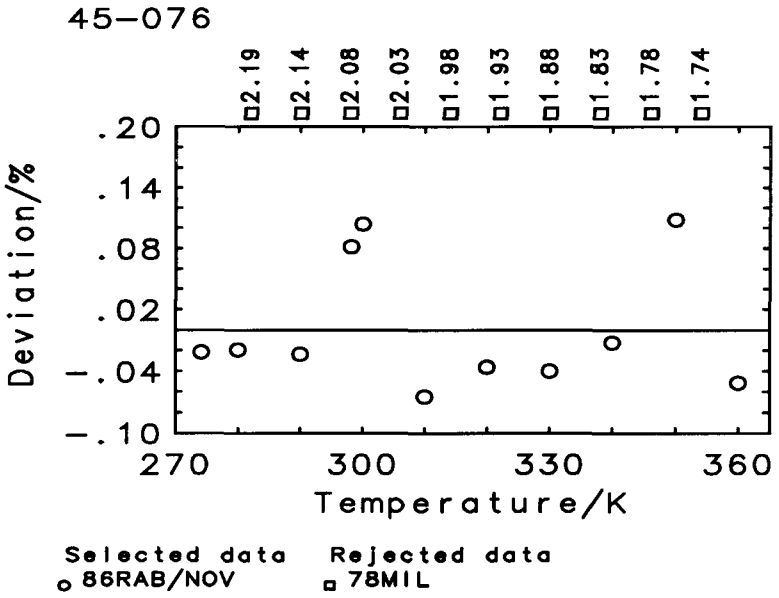
TABLE 45.76.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1}g^{-1}$)	1.528	1.545	1.560	1.563	1.580	1.598	1.616
C_p ($J K^{-1}mol^{-1}$)	296.7	300.1	302.9	303.5	306.9	310.3	313.7
Temp. (K)	340	350	360				
c_p ($J K^{-1}g^{-1}$)	1.633	1.651	1.668				
C_p ($J K^{-1}mol^{-1}$)	317.1	320.6	324.0				

TABLE 45.76.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	11	0.141	2.65–2	0.07	2.88–5	–5

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
274.2–360.0	765.00	1.19674	1.07132–2	2.39746+1	3.34212+1	IV



Name: Dimethyl 1,4–benzenedicarboxylate
Formula: $C_{10}H_{10}O_4$

CAS–RN: 120–61–6
Group No.: 45–077
Molar Mass: 194.19

TABLE 45.77.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
56SMI/DOL	N	416.0–463.0	eqn	0.50	99.978	anal	C_p	BSAO	55MAR/SMI
68ELL/CHR		423.4–466.3	4	2.00	99.93	melpt	C_p	BSAO	49HOR/STO

56SMI/DOL impurities water 0.017 %, nitrocompounds 0.005 %

TABLE 45.77.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56SMI/DOL	416.0–462.8	10	0.50	0.000	2.41–6	0.00	–7.63–7	0
				Rejected data				
68ELL/CHR	(9.57–1, 2.11, 9.46–1, 3)							

TABLE 45.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	10	0.000	2.70–6	0.00	–7.63–7	0
Temp. range K		A_1	A_2				Level of uncertainty
416.0–462.8		1.83208+1	5.99989				IV

TABLE 45.77.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460
c_p ($J K^{-1}g^{-1}$)	1.863	1.889	1.915	1.940	1.966
C_p ($J K^{-1}mol^{-1}$)	361.9	366.8	371.8	376.8	381.8

Name: Propyl benzoate
Formula: $C_{10}H_{12}O_2$

CAS–RN: 2315–68–6
Group No.: 45–078
Molar Mass: 164.20

TABLE 45.78.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	318.1–346.9	5S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.78.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.002	2.22–3	0.01	–2.29–6	0
Temp. range K		A_1	A_2				Level of uncertainty
318.1–346.9		1.40351+1	6.40520				V

TABLE 45.78.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c ($J K^{-1}g^{-1}$)	1.75	1.78	1.81	1.85
C ($J K^{-1}mol^{-1}$)	287	292	298	303

Name: Di–2–propenyl butanedioate
Formula: $C_{10}H_{14}O_4$

CAS–RN: 925–16–6
Group No.: 45–079
Molar Mass: 198.22

TABLE 45.79.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	320.0–348.4	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.79.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.018	2.61–2	0.06	1.91–5	0
Temp. range K		A_1	A_2				Level of uncertainty
320.0–348.4		2.46415+1	6.73774				V

TABLE 45.79.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.94	1.97	1.99	2.02
C_p ($J K^{-1} mol^{-1}$)	384	390	395	401

Name: Bis(2–methylpropyl) ethanedioate
Formula: $C_{10}H_{18}O_4$

CAS–RN: 2050–61–5
Group No.: 45–080
Molar Mass: 202.25

TABLE 45.80.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	318.4–346.8	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.80.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.030	4.23–2	0.09	4.83–5	0
Temp. range K		A_1	A_2				Level of uncertainty
318.4–346.8		2.40107+1	7.05585				V

TABLE 45.80.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.92	1.94	1.97	2.00
C_p ($J K^{-1} mol^{-1}$)	387	393	399	405

Name: Dipropyl butanedioate
Formula: $C_{10}H_{18}O_4$

CAS–RN: 925–15–5
Group No.: 45–081
Molar Mass: 202.25

TABLE 45.81.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	319.0–347.2	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.061	8.92–2	0.18	2.00–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
319.0–347.2		2.38750+1	7.45260				V

TABLE 45.81.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	1.96	1.99	2.02	2.05
C_p ($J K^{-1}mol^{-1}$)	397	403	409	415

Name: 1,2–Ethanediyl dibutanoate
Formula: $C_{10}H_{18}O_4$

CAS–RN: 105–72–6
Group No.: 45–082
Molar Mass: 202.25

TABLE 45.82.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86NIL/WAD	298.15	1.880	nosp	99.9	chrom	C_p	DDCT	71KON/SUU

Name: Hexyl butanoate
Formula: $C_{10}H_{20}O_2$

CAS–RN: 2639–63–6
Group No.: 45–083
Molar Mass: 172.27

TABLE 45.83.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80BAL/PET	N	200.0–370.0	18S	1.00	not specified		C_p	not specified	

80BAL/PET error of 0.3–1.0 % reported in 84VAS/PET

TABLE 45.83.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.115	4.59–2	0.12	7.88–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.0–370.0		5.96805+1	–2.64359+1	9.34610	–9.05074–1		IV

TABLE 45.83.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	1.784	1.786	1.792	1.801	1.813	1.827	1.845
C_p ($J K^{-1}mol^{-1}$)	307.2	307.6	308.6	310.2	312.3	314.8	317.8
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	1.864	1.871	1.885	1.909	1.928	1.933	1.959
C_p ($J K^{-1}mol^{-1}$)	321.1	322.3	324.8	328.8	332.2	333.0	337.4
Temp. (K)	320	330	340	350	360	370	
c_p ($J K^{-1}g^{-1}$)	1.985	2.012	2.040	2.068	2.095	2.122	
C_p ($J K^{-1}mol^{-1}$)	342.0	346.7	351.4	356.2	360.9	365.6	

TABLE 45.83.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.422	1.63–1	0.42	1.09–3	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.0–370.0	657.20	1.30151+1	1.51801+1	1.87072+1	2.78972		IV

Name: 3–Methylbutyl pentanoate
Formula: $C_{10}H_{20}O_2$

CAS–RN: 2050–09–1
Group No.: 45–084
Molar Mass: 172.27

TABLE 45.84.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*86SCH	310.3–345.5	8S	nosp	not specified		C_{avg}	DSIO	*86SCH

TABLE 45.84.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	8	8	0.002	2.62–3	0.01	–1.43–6	0
Temp. range K		A_1	A_2				Level of uncertainty
310.3–345.5		1.75954+1	7.58061				V

TABLE 45.84.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c ($J K^{-1}g^{-1}$)	1.98	2.02	2.06	2.09	2.13
C ($J K^{-1}mol^{-1}$)	342	348	354	361	367

Name: Octyl acetate
Formula: $C_{10}H_{20}O_2$

CAS-RN: 112-14-1
Group No.: 45-085
Molar Mass: 172.27

TABLE 45.85.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91DES/PAT	298.15	1.995	nosp	98.	anal	C_p	FSIT	71PIC/LED

Name: Ethyl 3-phenyl-2-propenoate
Formula: $C_{11}H_{12}O_2$

CAS-RN: 103-36-6
Group No.: 45-086
Molar Mass: 176.22

TABLE 45.86.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	316.1-379.6	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 45.86.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C	4	4	0.117	1.42-1	0.35	4.50-4	0

Temp. range K	A_1	A_2	Level of uncertainty
316.1-379.6	1.66936+1	6.32935	V

TABLE 45.86.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J\,K^{-1}g^{-1}$)	1.74	1.77	1.80	1.83	1.86	1.89	1.92
C ($J\,K^{-1}mol^{-1}$)	307	312	318	323	328	334	339

Name: Phenylmethyl 2-methyl-2-propenoate
Formula: $C_{11}H_{12}O_2$

CAS-RN: 2495-37-6
Group No.: 45-087
Molar Mass: 176.22

TABLE 45.87.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
58DVO	296.55	1.531	nosp	not specified		C_p	not specified	

Name: Ethyl benzenepropanoate
Formula: $C_{11}H_{14}O_2$

CAS–RN: 2021–28–5
Group No.: 45–088
Molar Mass: 178.23

TABLE 45.88.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	316.3–376.0	6S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 45.88.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C	6	6	0.003	3.18–3	0.01	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
316.3–376.0	9.55721	8.96674	V

TABLE 45.88.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J K^{-1} g^{-1}$)	1.78	1.83	1.87	1.91	1.95	1.99	2.04
C ($J K^{-1} mol^{-1}$)	318	325	333	340	348	355	363

Name: Methyl decanoate
Formula: $C_{11}H_{22}O_2$

CAS–RN: 110–42–9
Group No.: 45–089
Molar Mass: 186.29

TABLE 45.89.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.15	2.055	0.50	99.	chrom	C_p	BSIO	80FUC

Name: Diethyl 1,2–benzenedicarboxylate
Formula: $C_{12}H_{14}O_4$

CAS–RN: 84–66–2
Group No.: 45–090
Molar Mass: 222.24

TABLE 45.90.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67CHA/HOR	273.0–353.4	25	0.10	99.88	melpt	C_p	BSAO	65STE/BLA
79FUC	298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC

TABLE 45.90.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67CHA/HOR	273.0–353.4	25	0.10	0.628	2.75–2	0.06	3.31–5	–3
				Rejected data				
79FUC	(1.03, 2.39,–1.03, –1)							

TABLE 45.90.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	25	0.669	2.93–2	0.07	3.31–5	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–353.4		3.33731+1	1.42104	7.24336–1			II

TABLE 45.90.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.590	1.596	1.610	1.631	1.648	1.652	1.674
C_p (J K^{-1}mol^{-1})	353.3	354.7	357.8	362.4	366.2	367.1	372.0
Temp. (K)	320	330	340	350			
c_p (J K^{-1}g^{-1})	1.696	1.719	1.743	1.767			
C_p (J K^{-1}mol^{-1})	377.0	382.1	387.3	392.6			

TABLE 45.90.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	25	0.671	2.93–2	0.07	3.48–5	–2

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
273.0–353.4	760.20	–1.31657+1	4.66333	2.61784+1	9.29246	II

Name: Diethyl 1,4-benzenedicarboxylate
Formula: $C_{12}H_{14}O_4$

CAS-RN: 636-09-9
Group No.: 45-091
Molar Mass: 222.24

TABLE 45.91.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
56SMI/DOL	N	316.0–348.0	eqn	0.25	not specified		C_p	BSAO	55MAR/SMI

56SMI/DOL sample of low purity (premelting at 10 K)

TABLE 45.91.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.000	2.70–6	0.00	–1.43–6	0
Temp. range K		A_1	A_2				Level of uncertainty
316.0–348.2		2.23058+1	7.26929				V

TABLE 45.91.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p (J K^{-1}g^{-1})	1.70	1.73	1.76	1.79
C_p (J K^{-1}mol^{-1})	379	385	391	397

Name: 1,2,3–Propanetriyl tripropanoate
Formula: $C_{12}H_{20}O_6$

CAS–RN: 139–45–7
Group No.: 45–092
Molar Mass: 260.29

TABLE 45.92.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86NIL/WAD	298.15	1.849	nosp	99.9	chrom	C_p	DDCT	71KON/SUU

Name: Nonyl 2–propenoate
Formula: $C_{12}H_{22}O_2$

CAS–RN: 2664–55–3
Group No.: 45–093
Molar Mass: 198.31

TABLE 45.93.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
85KAR/ABD1	N	237.0–333.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD1 same data in 85KAR/SAI

TABLE 45.93.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.728	1.71–1	0.36	8.53–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
237.0–333.3		2.39985+1	3.48253	1.78206			VI

TABLE 45.93.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.79	1.84	1.89	1.95	1.96	2.00	2.06
C_p (J K^{-1}mol^{-1})	354	365	375	386	389	397	408
Temp. (K)	298.15	300	310	320	330		
c_p (J K^{-1}g^{-1})	2.11	2.12	2.18	2.24	2.30		
C_p (J K^{-1}mol^{-1})	418	420	432	444	456		

Name: Octyl 2–methyl–2–propenoate
Formula: $C_{12}H_{22}O_2$

CAS–RN: 2157–01–9
Group No.: 45–094
Molar Mass: 198.31

TABLE 45.94.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85KAR/ABD2 N	230.0–350.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD2 same data in 85KAR/SAI

TABLE 45.94.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.000	1.15–6	0.00	–2.93–7	0
Temp. range K		A_1	A_2				Level of uncertainty
230.0–350.0		3.00946+1	5.47870				VI

TABLE 45.94.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.79	1.81	1.84	1.86	1.88	1.89	1.90
C_p (J K^{-1}mol^{-1})	355	360	364	369	373	375	378
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.93	1.95	1.95	1.97	2.00	2.02	2.04
C_p (J K^{-1}mol^{-1})	382	386	387	391	396	401	405
Temp. (K)	350						
c_p (J K^{-1}g^{-1})	2.07						
C_p (J K^{-1}mol^{-1})	410						

Name: Bis(3–methylbutyl) ethanedioate
Formula: $C_{12}H_{22}O_4$

CAS–RN: 2051–00–5
Group No.: 45–095
Molar Mass: 230.30

TABLE 45.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	318.4–347.0	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.95.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.017	2.86–2	0.05	2.23–5	0
Temp. range K		A_1	A_2				Level of uncertainty
318.4–347.0		2.73490+1	8.29107				V

TABLE 45.95.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.95	1.98	2.01	2.04
C_p ($J\,K^{-1}mol^{-1}$)	448	455	462	469

Name: Bis(2–methylpropyl) butanedioate
Formula: $C_{12}H_{22}O_4$

CAS–RN: 925–06–4
Group No.: 45–096
Molar Mass: 230.30

TABLE 45.96.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	319.0–347.7	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.96.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.007	1.18–2	0.02	5.72–6	0
Temp. range K		A_1	A_2				Level of uncertainty
319.0–347.7		2.97768+1	7.81683				V

TABLE 45.96.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.98	2.01	2.03	2.06
C_p ($J\,K^{-1}mol^{-1}$)	456	462	469	475

Name: Dibutyl butanedioate
Formula: $C_{12}H_{22}O_4$

CAS-RN: 141-03-7
Group No.: 45-097
Molar Mass: 230.30

TABLE 45.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89KHO/PUL	250.0–300.0	8S	1.00	97.16	melpt	C_p	BSAO	89KHO/PUL
89KHO/PUL	310.0–400.0	10S	1.50	97.16	melpt	C_p	BDHT	86MER/BEN

TABLE 45.97.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89KHO/PUL	250.0–300.0	8	1.00	0.094	4.93–2	0.09	–1.57–2	0
89KHO/PUL	310.0–400.0	10	1.50	0.061	4.99–2	0.09	2.84–2	4

TABLE 45.97.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.085	5.44–2	0.10	8.83–3	4

Temp. range K	A_1	A_2	A_3	Level of uncertainty
250.0–400.0	5.60228+1	–6.54148	1.80387	V

TABLE 45.97.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.84	1.85	1.86	1.86	1.87	1.89	1.90
C_p (J K^{-1}mol^{-1})	424	426	428	429	431	434	437
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.90	1.92	1.93	1.95	1.97	1.99	2.02
C_p (J K^{-1}mol^{-1})	438	441	445	450	454	459	464
Temp. (K)	370	380	390	400			
c_p (J K^{-1}g^{-1})	2.04	2.07	2.09	2.12			
C_p (J K^{-1}mol^{-1})	470	476	482	488			

Name: Decyl acetate
Formula: $C_{12}H_{24}O_2$

CAS-RN: 112-17-4
Group No.: 45-098
Molar Mass: 200.32

TABLE 45.98.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91DES/PAT	298.15	2.315	nosp	99.	anal	C_p	FSIT	71PIC/LED

Name: Nonyl 2–methyl–2–propenoate
Formula: $C_{13}H_{24}O_2$

CAS–RN: 2696–43–7
Group No.: 45–099
Molar Mass: 212.33

TABLE 45.99.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89GUS/BAI	244.5–314.8	13	0.40	99.94	chrom	C_p	BSAO	77KU/COM

TABLE 45.99.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.338	6.77–2	0.14	1.45–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
244.5–314.8		6.00194+1	–1.28315+1	3.22953			IV

TABLE 45.99.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.873	1.884	1.899	1.916	1.921	1.935	1.957
C_p (J K^{-1}mol^{-1})	397.6	400.1	403.2	406.7	408.0	410.8	415.5
Temp. (K)	298.15	300	310				
c_p (J K^{-1}g^{-1})	1.976	1.981	2.008				
C_p (J K^{-1}mol^{-1})	419.6	420.6	426.3				

Name: Decyl 2–methyl–2–propenoate
Formula: $C_{14}H_{26}O_2$

CAS–RN: 3179–47–3
Group No.: 45–100
Molar Mass: 226.36

TABLE 45.100.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85KAR/ABD2	N	251.0–350.0	eqn	0.50	not specified		C_p	BSAO	82KAR/IGA

85KAR/ABD2 same data in 85KAR/SAI

TABLE 45.100.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	2.34–6	0.00	1.14–6	0
Temp. range K		A_1	A_2				Level of uncertainty
251.0–350.0		2.99117+1	8.23571				VI

TABLE 45.100.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.89	1.92	1.93	1.95	1.98	2.00	2.01
C_p (J K^{-1}mol^{-1})	427	434	436	440	447	453	454
Temp. (K)	310	320	330	340	350		
c_p (J K^{-1}g^{-1})	2.04	2.07	2.10	2.13	2.16		
C_p (J K^{-1}mol^{-1})	461	468	475	482	488		

Name: Bis(3–methylbutyl) butanedioate
Formula: $C_{14}H_{26}O_4$

CAS–RN: 818–04–2
Group No.: 45–101
Molar Mass: 258.36

TABLE 45.101.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	319.1–347.9	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 45.101.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.047	9.00–2	0.14	1.58–4	–3
Temp. range K		A_1	A_2				Level of uncertainty
319.1–347.9		3.28326+1	9.21307				V

TABLE 45.101.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p (J K^{-1}g^{-1})	2.01	2.04	2.06	2.09
C_p (J K^{-1}mol^{-1})	518	526	533	541

Name: 1,2,3–Propanetriyl tributanoate
Formula: $C_{15}H_{26}O_6$

CAS–RN: 60–01–5
Group No.: 45–102
Molar Mass: 302.37

TABLE 45.102.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76PHI/MAT	N	313.0–413.0	5	nosp	not specified		C_p	BDHT	73PER/COM
86NIL/WAD		298.1	1	nosp	99.	chrom	C_p	DDCT	71KON/SUU

76PHI/MAT reproducibility given as 5 %

TABLE 45.102.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76PHI/MAT	313.0–413.0	5	5.00#	0.463	1.73	2.31	2.50–1	–1
86NIL/WAD	298.1	1	0.30#	0.015	3.08–3	0.00	–3.08–3	0

TABLE 45.102.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.517	1.94	2.59	2.08–1	–1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–413.0		3.26021+1	1.14667+1				VI

TABLE 45.102.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.84	1.87	1.91	1.94	1.97	2.00	2.03
C_p (J K^{-1}mol^{-1})	557	567	576	586	595	605	614
Temp. (K)	370	380	390	400	410		
c_p (J K^{-1}g^{-1})	2.06	2.09	2.13	2.16	2.19		
C_p (J K^{-1}mol^{-1})	624	633	643	652	662		

Name: Methyl tetradecanoate
Formula: $C_{15}H_{30}O_2$

CAS–RN: 124–10–7
Group No.: 45–103
Molar Mass: 242.40

TABLE 45.103.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC	298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC
91DES/PAT	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 45.103.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79FUC	298.1	1	0.50	1.504	4.57–1	0.75	4.57–1	1
91DES/PAT	298.1	1	0.50#	1.482	4.44–1	0.74	–4.44–1	–1

TABLE 45.103.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	2.111	6.37–1	1.06	6.73–3	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		6.03282+1					IV

TABLE 45.103.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.069
C_p (J K^{-1}mol^{-1})	501.6

Name: Dibutyl 1,2–benzenedicarboxylate
Formula: $C_{16}H_{22}O_4$

CAS–RN: 84–74–2
Group No.: 45–104
Molar Mass: 278.35

TABLE 45.104.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70MAR/RAB	N	173.5–360.0	5S	0.30	not specified		C_p	BSAO	56POP/KOL
85RAB/NOV		173.9–300.1	40	nosp	99.7	chrom	C_p	BSAO	66NIK/LEB

70MAR/RAB same data in 69RAB/MAR at 300 K and 360 K

TABLE 45.104.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70MAR/RAB	200.0–360.0	4	0.30	0.271	4.39–2	0.08	9.30–3	–2
85RAB/NOV	177.1–300.1	37	0.50#	0.835	2.13–1	0.42	–9.81–4	3

TABLE 45.104.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	41	0.839	2.13–1	0.42	2.26–5	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
177.1–360.0		9.35517+1	–5.27527+1	2.03356+1	–2.25650		III

TABLE 45.104.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.533	1.531	1.533	1.540	1.550	1.563	1.580
C_p (J K^{-1}mol^{-1})	426.7	426.2	426.8	428.6	431.5	435.2	439.7
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.598	1.619	1.641	1.649	1.665	1.689	1.710
C_p (J K^{-1}mol^{-1})	444.9	450.7	456.9	458.9	463.5	470.2	475.9
Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.714	1.739	1.764	1.787	1.810	1.831	1.849
C_p (J K^{-1}mol^{-1})	477.2	484.1	490.9	497.5	503.7	509.5	514.8

TABLE 45.104.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	41	0.812	2.03–1	0.40	6.17–3	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
177.1–360.0	790.00	5.20734+4	7.87447+3	–7.85938+3	4.47831+4	1.47757+4	1.74564+4	III

Name: Dibutyl decanedioate
Formula: $C_{18}H_{34}O_4$

CAS-RN: 109–43–3
Group No.: 45–105
Molar Mass: 314.47

TABLE 45.105.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	312.0–412.0	5	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.105.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.438	1.83	2.19	5.04–2	1
Temp. range K		A_1	A_2				Level of uncertainty
312.0–412.0		2.81891+1	1.46075+1				VI

TABLE 45.105.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.94	1.98	2.02	2.06	2.10	2.14	2.17
C_p (J K^{-1}mol^{-1})	611	623	635	647	659	672	684
Temp. (K)	380	390	400	410			
c_p (J K^{-1}g^{-1})	2.21	2.25	2.29	2.33			
C_p (J K^{-1}mol^{-1})	696	708	720	732			

Name: 1,2,3–Propanetriyl ester hexanoic acid
Formula: $C_{21}H_{38}O_6$

CAS–RN: 621–70–5
Group No.: 45–106
Molar Mass: 386.53

TABLE 45.106.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	313.0–413.0	5	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.106.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.499	2.35	2.49	7.06–2	1
Temp. range K		A_1	A_2				Level of uncertainty
313.0–413.0		4.90790+1	1.29102+1				VI

TABLE 45.106.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	1.92	1.94	1.97	2.00	2.03	2.06	2.08
C_p ($J\,K^{-1}mol^{-1}$)	741	752	762	773	784	794	805
Temp. (K)	380	390	400	410			
c_p ($J\,K^{-1}g^{-1}$)	2.11	2.14	2.17	2.19			
C_p ($J\,K^{-1}mol^{-1}$)	816	827	837	848			

Name: Bis(2–ethylhexyl) hexanedioate
Formula: $C_{22}H_{42}O_4$

CAS–RN: 103–23–1
Group No.: 45–107
Molar Mass: 370.57

TABLE 45.107.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
85OVC/MOS	180.0–300.0	7S	0.20	99. chrom	C_p	BSAO	76LEB/LIT

TABLE 45.107.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.348	5.44–2	0.07	3.92–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.0–300.0		1.30980+2	–6.83667+1	2.70168+1	–3.13576		III

TABLE 45.107.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.731	1.730	1.733	1.739	1.749	1.761	1.776
C_p (J K^{-1}mol^{-1})	641.6	641.1	642.1	644.5	648.1	652.7	658.2
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.793	1.812	1.831	1.838	1.852	1.872	1.889
C_p (J K^{-1}mol^{-1})	664.5	671.4	678.6	681.0	686.2	693.8	700.1
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.893						
C_p (J K^{-1}mol^{-1})	701.5						

Name: Dihexyl decanedioate
Formula: $C_{22}H_{42}O_4$

CAS-RN: 2449-10-7
Group No.: 45-108
Molar Mass: 370.57

TABLE 45.108.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
75PHI/WAL		303.1–393.1	7S	nosp	not specified	C_p	BDHT	73PER/COM
76PHI/MAT	N	303.0–414.0	12	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.108.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75PHI/WAL	303.1–393.1	7	5.00#	0.165	7.46–1	0.82	–5.61–2	–1
76PHI/MAT	303.0–414.0	12	5.00#	0.311	1.48	1.56	8.55–2	0

TABLE 45.108.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.282	1.33	1.41	3.33–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
303.0–414.0		2.85666+1	1.84936+1				VI

TABLE 45.108.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.89	1.93	1.97	2.01	2.05	2.09	2.13
C_p (J K^{-1}mol^{-1})	699	714	730	745	760	776	791
Temp. (K)	370	380	390	400	410		
c_p (J K^{-1}g^{-1})	2.18	2.22	2.26	2.30	2.34		
C_p (J K^{-1}mol^{-1})	806	822	837	853	868		

Name: Butyl octadecanoate
Formula: $C_{22}H_{44}O_2$

CAS-RN: 123-95-5
Group No.: 45-109
Molar Mass: 340.59

TABLE 45.109.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86KAL/JAC	300.5–304.8	5	0.20	99.99	melpt	C_p	BSAO	80KAL/JED

TABLE 45.109.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	5	4	2.223	3.87–1	0.44	1.71–3	–2

Temp. range K	A_1	A_2	Level of uncertainty
301.8–304.8	–9.38329+1	5.94258+1	IV

TABLE 45.109.4. Recommended values of heat capacities

Temp. (K)	300
c_p (J K^{-1}g^{-1})	2.061
C_p (J K^{-1}mol^{-1})	702.1

Name: Bis(2-ethylhexyl)-1,2-benzenedicarboxylate
Formula: $C_{24}H_{38}O_4$

CAS-RN: 117-81-7
Group No.: 45-110
Molar Mass: 390.56

TABLE 45.110.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70MAR/RAB	N	182.5–360.0	5S	0.30	not specified		C_p	BSAO	56POP/KOL
85RAB/NOV		184.4–300.2	38	nosp	99.7	chrom	C_p	BSAO	66NIK/LEB

70MAR/RAB same data in 69RAB/MAR at 300 K and 360 K

TABLE 45.110.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
			Selected data					
70MAR/RAB	200.0–360.0	4	0.30	0.369	9.35–2	0.11	3.82–2	0
85RAB/NOV	190.0–300.2	35	0.50#	0.243	9.73–2	0.12	–1.18–2	–3

TABLE 45.110.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	43	39	0.273	1.02–1	0.13	–6.69–3	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
190.0–360.0		1.31946+2	–6.77009+1	2.52562+1	–2.64008		III

TABLE 45.110.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.626	1.627	1.633	1.642	1.654	1.670	1.688
C_p (J K^{-1}mol^{-1})	635.1	635.6	637.8	641.3	646.2	652.2	659.3
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.708	1.731	1.738	1.755	1.780	1.802	1.807
C_p (J K^{-1}mol^{-1})	667.3	676.0	678.9	685.4	695.3	703.7	705.6
Temp. (K)	310	320	330	340	350	360	
c_p (J K^{-1}g^{-1})	1.834	1.861	1.888	1.915	1.941	1.966	
C_p (J K^{-1}mol^{-1})	716.2	726.8	737.5	748.0	758.2	768.0	

Name: 2,3–Bis(acetyloxy)propyl ester octadecanoic acid
Formula: $C_{25}H_{46}O_6$

CAS–RN: 33599–07–4
Group No.: 45–111
Molar Mass: 442.64

TABLE 45.111.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
55WAR/VIC	334.4–370.0	10	1.00	98.	melpt	C_p	BSAO	44BAI/TOD

TABLE 45.111.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	1.640	2.03	1.64	4.78–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
334.5–370.0		5.29227+3	–2.91516+3	4.10655+2			V

TABLE 45.111.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.71	2.40	2.25	2.25	2.41
C_p (J K^{-1}mol^{-1})	1200	1060	996	996	1060

Name: Bis(2–ethylhexyl) nonanedioate
Formula: $C_{25}H_{48}O_4$

CAS–RN: 103–24–2
Group No.: 45–112
Molar Mass: 412.65

TABLE 45.112.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83BAB/RAB	N	170.5–336.0	33	0.20	98.	chrom	C_p	BSAO	76LEB/LIT

83BAB/RAB data below 208 K glass phase

TABLE 45.112.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	33	1.062	1.97–1	0.21	7.01–4	5

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
170.5–250.0	6.56880+1	4.21852+1	–2.52225+1	4.92911	III
250.0–336.0	2.67221+2	–1.99654+2	7.15134+1	–7.96901	III

TABLE 45.112.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p ($J K^{-1}g^{-1}$)	1.788	1.786	1.785	1.785	1.787	1.791	1.798
C_p ($J K^{-1}mol^{-1}$)	737.7	737.1	736.6	736.7	737.4	739.2	742.1
Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	1.809	1.824	1.843	1.866	1.874	1.892	1.920
C_p ($J K^{-1}mol^{-1}$)	746.6	752.7	760.7	770.2	773.5	780.9	792.3
Temp. (K)	298.15	300	310	320	330	340	
c_p ($J K^{-1}g^{-1}$)	1.943	1.949	1.977	2.005	2.030	2.053	
C_p ($J K^{-1}mol^{-1}$)	801.9	804.1	815.9	827.3	837.8	847.1	

Name: Dioctyl decanedioate
Formula: $C_{26}H_{50}O_4$

CAS–RN: 2432–87–3
Group No.: 45–113
Molar Mass: 426.68

TABLE 45.113.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76PHI/MAT	N	318.0–393.0	4	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.113.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.200	1.07	1.00	1.10–2	2
Temp. range K		A_1	A_2				Level of uncertainty
318.0–393.0		7.02359+1	9.96586				VI

TABLE 45.113.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.99	2.01	2.03	2.05	2.07	2.09	2.11
C_p (J K^{-1}mol^{-1})	849	857	866	874	882	891	899
Temp. (K)	390						
c_p (J K^{-1}g^{-1})	2.13						
C_p (J K^{-1}mol^{-1})	907						

Name: 1,2,3–Propanetriyl ester octanoic acid
Formula: $C_{27}H_{50}O_6$

CAS–RN: 538–23–8
Group No.: 45–114
Molar Mass: 470.69

TABLE 45.114.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	338.0–413.0	3	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.114.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.321	1.88	1.61	1.96–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
338.0–413.0		7.68542+1	1.01485+1				VI

TABLE 45.114.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	1.97	1.99	2.00	2.02	2.04	2.06	2.07
C_p (J K^{-1}mol^{-1})	926	934	943	951	960	968	977
Temp. (K)	410						
c_p (J K^{-1}g^{-1})	2.09						
C_p (J K^{-1}mol^{-1})	985						

Name: Didecyl decanedioate
Formula: $C_{30}H_{58}O_4$

CAS–RN: 2432–89–5
Group No.: 45–115
Molar Mass: 482.79

TABLE 45.115.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	368.0–403.0	3	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.115.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.470	3.03	2.35	4.89–2	1

Temp. range K	A_1	A_2	Level of uncertainty
368.0–403.0	–4.24360	3.38075+1	VI

TABLE 45.115.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400
c_p (J $K^{-1}g^{-1}$)	2.08	2.14	2.20	2.26
C_p (J $K^{-1}mol^{-1}$)	1000	1030	1060	1090

Name: 1,2,3–Propanetriyl ester decanoic acid
Formula: $C_{33}H_{62}O_6$

CAS–RN: 621–71–6
Group No.: 45–116
Molar Mass: 554.85

TABLE 45.116.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	313.0–388.0	3	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.116.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.398	2.83	1.99	3.65–2	–1

Temp. range K	A_1	A_2	Level of uncertainty
313.0–388.0	9.26622+1	1.32124+1	VI

TABLE 45.116.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	2.00	2.02	2.04	2.06	2.08	2.10	2.12
C_p ($J K^{-1}mol^{-1}$)	1110	1120	1130	1140	1150	1170	1180
Temp. (K)	380	390					
c_p ($J K^{-1}g^{-1}$)	2.14	2.16					
C_p ($J K^{-1}mol^{-1}$)	1190	1200					

Name: Didodecyl decanedioate
Formula: $C_{34}H_{66}O_4$

CAS-RN: 2432-88-4
Group No.: 45-117
Molar Mass: 538.90

TABLE 45.117.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76PHI/MAT	N	368.0-408.0	3	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.117.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.014	9.87-2	0.07	2.04-5	-1
Temp. range K		A_1	A_2				Level of uncertainty
368.0-408.0		3.67630+1	2.65252+1				VI

TABLE 45.117.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410
c_p ($J K^{-1}g^{-1}$)	2.08	2.12	2.16	2.20	2.25
C_p ($J K^{-1}mol^{-1}$)	1120	1140	1170	1190	1210

Name: 1,6-Hexanediyldihexyl ester decanedioic acid
Formula: $C_{38}H_{70}O_8$

CAS-RN: 55205-81-7
Group No.: 45-118
Molar Mass: 654.97

TABLE 45.118.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75PHI/WAL	N	328.1-408.1	4S	nosp	not specified		C_p	BDHT	73PER/COM
76PHI/MAT		328.0-408.0	4S	5.00	not specified		C_p	BDHT	73PER/COM

75PHI/WAL misprint in the original source

TABLE 45.118.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75PHI/WAL	328.1–408.1	4	5.00#	0.020	1.65–1	0.10	–1.18–1	–2
76PHI/MAT	328.0–408.0	4	5.00	0.032	2.63–1	0.16	1.19–1	2

TABLE 45.118.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.034	2.78–1	0.17	6.08–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
328.0–408.1		2.42622+2	–5.89282+1	9.85248			VI

TABLE 45.118.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p (J $K^{-1}g^{-1}$)	1.97	1.98	1.99	2.01	2.02	2.04	2.06
C_p (J $K^{-1}mol^{-1}$)	1290	1300	1310	1320	1330	1340	1350
Temp. (K)	400	410					
c_p (J $K^{-1}g^{-1}$)	2.09	2.12					
C_p (J $K^{-1}mol^{-1}$)	1370	1390					

Name: Ditetradecyl decanedioate
Formula: $C_{38}H_{74}O_4$

CAS–RN: 26719–47–1
Group No.: 45–119
Molar Mass: 595.00

TABLE 45.119.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76PHI/MAT	N	343.0–433.0	5	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.119.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.183	1.52	0.91	1.14–2	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
343.0–433.0		–2.39857+2	1.84655+2	–2.06822+1			VI

TABLE 45.119.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1}g^{-1}$)	2.08	2.14	2.19	2.24	2.28	2.32	2.35
C_p ($J K^{-1}mol^{-1}$)	1240	1270	1300	1330	1360	1380	1400
Temp. (K)	410	420	430				
c_p ($J K^{-1}g^{-1}$)	2.37	2.39	2.40				
C_p ($J K^{-1}mol^{-1}$)	1410	1420	1430				

Name: 1,2,3–Propanetriyl ester dodecanoic acid
Formula: $C_{39}H_{74}O_6$

CAS–RN: 538–24–9
Group No.: 45–120
Molar Mass: 639.01

TABLE 45.120.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47CHA/SIN		330.9–370.2	6	nosp	98.	estim	C_p	BSAO	44BAI/TOD
76PHI/MAT	N	323.0–398.0	4	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.120.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CHA/SIN	330.9–370.2	6	1.50#	0.107	2.68–1	0.16	9.13–4	–2
				Rejected data				
76PHI/MAT	(1.04+1, 6.68,–1.04+1, –1)							

TABLE 45.120.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	6	0.131	3.28–1	0.20	9.13–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
330.9–370.2		1.00676+2	1.87393+1				V

TABLE 45.120.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	2.11	2.14	2.16	2.19	2.21
C_p ($J K^{-1}mol^{-1}$)	1350	1370	1380	1400	1410

Name: Cholest–5–en–3–ol (3β) tetradecanoate
Formula: $C_{41}H_{72}O_2$

CAS–RN: 1989–52–2
Group No.: 45–121
Molar Mass: 597.02

TABLE 45.121.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67BAR/POR	N	364.6–373.1	3	nosp	99.9	anal	C_p	BDHT	73PER/COM

67BAR/POR data from a graph only

TABLE 45.121.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.220	1.08	0.66	4.65–3	–1

Temp. range K	A_1	A_2	Level of uncertainty
364.6–373.1	–6.18179+1	6.10844+1	V

TABLE 45.121.4. Recommended values of heat capacities

Temp. (K)	360	370
c_p (J K^{-1}g^{-1})	2.20	2.29
C_p (J K^{-1}mol^{-1})	1310	1370

Name: 1,2,3,4,5,6–Benzenehexayl ester hexanoic acid
Formula: $C_{42}H_{66}O_{12}$

CAS–RN: 65201–69–6
Group No.: 45–122
Molar Mass: 762.98

TABLE 45.122.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80SOR/TSU	371.9–391.8	6	nosp	99.98	melpt	C_p	BSAO	83YOS/SOR1

TABLE 45.122.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.086	4.98–2	0.03	1.02–5	–2

Temp. range K	A_1	A_2	Level of uncertainty
371.9–391.8	1.64338+2	7.50519	II

TABLE 45.122.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_p (J K^{-1}g^{-1})	2.093	2.102	2.110
C_p (J K^{-1}mol^{-1})	1597	1604	1610

Name: Dihexadecyl decanedioate
Formula: $C_{42}H_{82}O_4$

CAS–RN: 26719–48–2
Group No.: 45–123
Molar Mass: 651.11

TABLE 45.123.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	353.0–418.0	4	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.123.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.346	3.06	1.73	5.52–2	0

Temp. range K	A_1	A_2	Level of uncertainty
353.0–418.0	6.90913+1	2.93692+1	VI

TABLE 45.123.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.19	2.23	2.27	2.31	2.34	2.38	2.42
C_p (J K^{-1}mol^{-1})	1430	1450	1480	1500	1530	1550	1580

Temp. (K)	420
c_p (J K^{-1}g^{-1})	2.46
C_p (J K^{-1}mol^{-1})	1600

Name: 1,2,3–Propanetriyl ester tetradecanoic acid
Formula: $C_{45}H_{86}O_6$

CAS–RN: 555–45–3
Group No.: 45–124
Molar Mass: 723.17

TABLE 45.124.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
47CHA/SIN		331.5–365.0	6	nosp	98. estim	C_p	BSAO	44BAI/TOD
76PHI/MAT	N	333.0–433.0	5	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.124.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CHA/SIN	331.5–365.0	6	1.50#	0.089	2.54–1	0.13	7.02–4	–2
				Rejected data				
76PHI/MAT	(8.98, 4.97,–8.98, –2)							

TABLE 45.124.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	6	0.126	3.60–1	0.19	7.02–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
331.5–365.0		4.47542+2	–1.69547+2	2.74524+1			V

TABLE 45.124.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370
c_p (J K^{-1}g^{-1})	2.15	2.17	2.19	2.22	2.25
C_p (J K^{-1}mol^{-1})	1550	1570	1580	1600	1630

Name: Dioctadecyl decanedioate
Formula: $C_{46}H_{90}O_4$

CAS-RN: 3072-03-5
Group No.: 45-125
Molar Mass: 707.22

TABLE 45.125.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
76PHI/MAT	N	353.0–453.0	5	nosp	not specified	C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.125.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.468	4.34	2.34	1.20–1	–3
Temp. range K		A_1	A_2				Level of uncertainty
353.0–453.0		1.61983+2	5.38818				VI

TABLE 45.125.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	2.13	2.13	2.14	2.15	2.15	2.16	2.16
C_p (J K^{-1}mol^{-1})	1500	1510	1510	1520	1520	1530	1530
Temp. (K)	420	430	440	450			
c_p (J K^{-1}g^{-1})	2.17	2.18	2.18	2.19			
C_p (J K^{-1}mol^{-1})	1530	1540	1540	1550			

Name: 1,2,3,4,5,6–Benzenehexayl ester heptanoic acid
Formula: $C_{48}H_{78}O_{12}$

CAS–RN: 65201–70–9
Group No.: 45–126
Molar Mass: 847.14

TABLE 45.126.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81SOR/SUG	360.1–390.6	9	nosp	99.94	melpt	C_p	BSAO	83YOS/SOR1

TABLE 45.126.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.173	1.16–1	0.05	5.26–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
360.0–390.6		1.12218+3	–4.66709+2	6.05217+1			II

TABLE 45.126.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390
c_p ($J\,K^{-1}g^{-1}$)	2.222	2.197	2.185	2.184
C_p ($J\,K^{-1}mol^{-1}$)	1882	1862	1851	1850

Name: 1,2,3–Propanetriyl ester hexadecanoic acid
Formula: $C_{51}H_{98}O_6$

CAS–RN: 555–44–2
Group No.: 45–127
Molar Mass: 807.34

TABLE 45.127.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47CHA/SIN		338.8–369.1	6	nosp	98.	estim	C_p	BSAO	44BAI/TOD
76PHI/MAT	N	343.0–418.0	4	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.127.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CHA/SIN	338.8–369.1	6	1.50#	0.061	1.95–1	0.09	3.48–4	–2
				Rejected data				
76PHI/MAT	(1.14+1, 5.60,–1.14+1, –2)							

TABLE 45.127.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	6	0.075	2.39–1	0.11	3.48–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
338.8–369.1		1.21478+2	2.64329+1				V

TABLE 45.127.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_p (J K^{-1}g^{-1})	2.18	2.20	2.23	2.26
C_p (J K^{-1}mol^{-1})	1760	1780	1800	1820

Name: 1,2,3,4,5,6–Benzenehexayl ester octanoic acid
Formula: $C_{54}H_{90}O_{12}$

CAS–RN: 65201–71–0
Group No.: 45–128
Molar Mass: 931.30

TABLE 45.128.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
82SOR/YOS	358.4–390.1	9	nosp	99.77	melpt	C_p	BSAO	83YOS/SOR1

TABLE 45.128.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.127	1.07–1	0.04	4.07–5	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
358.4–390.1		1.66533+3	–7.07540+2	9.00805+1			II

TABLE 45.128.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390
c_p (J K^{-1}g^{-1})	2.550	2.505	2.477	2.465
C_p (J K^{-1}mol^{-1})	2375	2333	2307	2295

Name:10,19,28,37–Tetraoxodihexyl ester 11,18,29,36–tetraoxahexatetracosanedioic acid
Formula: $C_{54}H_{98}O_{12}$

CAS–RN: 55205–82–8
Group No.: 45–129
Molar Mass: 939.36

TABLE 45.129.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75PHI/WAL	N	333.1–433.1	4S	nosp	not specified		C_p	BDHT	73PER/COM
76PHI/MAT		333.0–433.0	4S	5.00	not specified		C_p	BDHT	73PER/COM

75PHI/WAL misprint in the original source

TABLE 45.129.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
75PHI/WAL	333.1–433.1	4	5.00#	0.153	1.74	0.76	6.35–1	–1
76PHI/MAT	333.0–433.0	4	5.00	0.073	8.08–1	0.36	–6.02–1	–3

TABLE 45.129.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.138	1.56	0.69	1.60–2	–4
Temp. range K		A_1	A_2				Level of uncertainty
333.0–433.1		1.92207+2	8.49388				VI

TABLE 45.129.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p (J K^{-1}g^{-1})	1.95	1.96	1.96	1.97	1.98	1.99	1.99
C_p (J K^{-1}mol^{-1})	1830	1840	1850	1850	1860	1870	1870
Temp. (K)	400	410	420	430			
c_p (J K^{-1}g^{-1})	2.00	2.01	2.02	2.02			
C_p (J K^{-1}mol^{-1})	1880	1890	1890	1900			

Name: 1,2,3–Propanetriyl ester octadecanoic acid
Formula: $C_{57}H_{110}O_6$

CAS–RN: 555–43–1
Group No.: 45–130
Molar Mass: 891.50

TABLE 45.130.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
47CHA/SIN		346.5–371.6	6	nosp	98.	estim	C_p	BSAO	44BAI/TOD
76PHI/MAT	N	353.0–453.0	5	nosp	not specified		C_p	BDHT	73PER/COM

76PHI/MAT reproducibility given as 5 %

TABLE 45.130.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47CHA/SIN	346.5–371.6	6	1.50#	0.154	5.55–1	0.23	1.99–2	–1
76PHI/MAT	353.0–453.0	5	5.00#	0.315	3.94	1.58	–1.12–1	–3

TABLE 45.130.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.266	2.97	1.19	–4.01–2	–4
Temp. range K		A_1	A_2				Level of uncertainty
346.5–453.0		1.66785+2	2.03516+1				V

TABLE 45.130.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1} g^{-1}$)	2.22	2.24	2.26	2.28	2.30	2.31	2.33
C_p ($J K^{-1} mol^{-1}$)	1980	2000	2010	2030	2050	2060	2080
Temp. (K)	420	430	440	450			
c_p ($J K^{-1} g^{-1}$)	2.35	2.37	2.39	2.41			
C_p ($J K^{-1} mol^{-1}$)	2100	2110	2130	2150			

46. Heterocyclic Oxygen Compounds

The family of heterocyclic oxygen compounds contains 26 compounds of which five were measured at one temperature only. The compounds of this group were investigated for three reasons: they are of interest to polymer technology, they are constituents of coal and other fossil fuels, and they have structures of (such as: crown ethers) of interest for theoretical considerations. Most measurements are of good quality and were performed over a wide temperature range.

The data of 6 heterocyclic oxygen compounds present in coal were thoroughly investigated at BMB (52GUT/SCO, 73GOO/FIN), and latter at NIPER (86CHI/NGU, 90CHI/ARC, 90CHI/GAM); the reported uncertainty of 0.1 to 0.2 % seems to be realistic. The same is valid for two measurements at UMAA (65CAR/WES1, 70WES/WON) and at UOTO (80NAK/SUG) on structurally important compounds. Good quality data emerged from the studies on oxirane and tetrahydrofuran from CIUG (77LEB/EVS1, 78LEB/RAB) which are for the former compound in excellent agreement with the data from UCB (49GIA/GOR). Methyloxirane was studied up to 301 K at DCM (64OET) showing data of good quality; these results were extended up to 325 K using a data set from DICP (82TAN/ZHO) which differed by about 1 % from the former data. Measurements were carried out at USE (66BEA/CLE, 69CLE/MEL1-4) for five compounds with two and more oxygen atoms in a ring having an uncertainty of 1-2 %; these data have applications to polymerization processes.

The compound studied most frequently in this family is 1,4-dioxane. Most sources report the data at one only temperature and are related to studies of mixtures which report limiting values for individual components. The PhD thesis (61ROU) from JHUB contains a large number of data points which cover a limited temperature interval (estimated measurement error near 1 %).

Name: Oxirane
Formula: C_2H_4O

CAS-RN: 75-21-8
Group No.: 46-001
Molar Mass: 44.05

TABLE 46.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
49GIA/GOR	166.0–283.9	22	0.20	99.98	melpt	C_p	BSIO	37GIA/EGA
77LEB/EVS1	160.7–283.7	7S	nosp	not specified		C_p	BSAO	76LEB/LIT

TABLE 46.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
49GIA/GOR	166.0–283.9	22	0.20	0.579	1.16–2	0.12	1.87–4	0
77LEB/EVS1	160.7–283.7	7	0.30#	0.260	7.93–3	0.08	–1.12–3	1

TABLE 46.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	29	0.561	1.16–2	0.12	–1.28–4	1
C_{sat}	29	29	0.565	1.17–2	0.12	–1.56–4	1

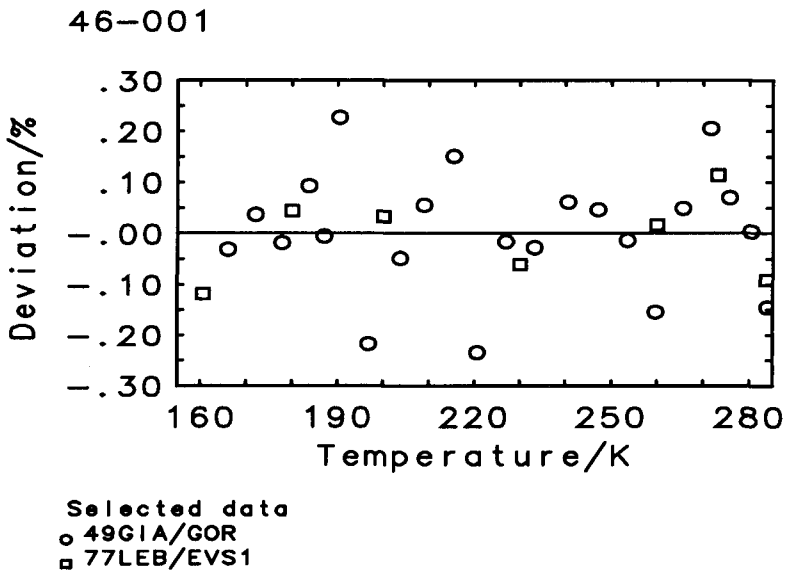
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
160.7–283.9	1.71467+1	–8.79031	3.25173	–3.47347–1	II
160.7–283.9	1.73432+1	–9.08783	3.40052	–3.71917–1	II

TABLE 46.1.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.867	1.856	1.850	1.849	1.852	1.859	1.869
C_p (J K^{-1}mol^{-1})	82.27	81.77	81.49	81.43	81.57	81.88	82.35
c_{sat} (J K^{-1}g^{-1})	1.867	1.856	1.850	1.849	1.852	1.859	1.869
C_{sat} (J K^{-1}mol^{-1})	82.27	81.76	81.49	81.43	81.57	81.88	82.35
Temp. (K)	240	250	260	270	273.15	280	
c_p (J K^{-1}g^{-1})	1.883	1.900	1.919	1.940	1.948	1.963	
C_p (J K^{-1}mol^{-1})	82.96	83.70	84.55	85.48	85.79	86.49	
c_{sat} (J K^{-1}g^{-1})	1.883	1.900	1.919	1.939	1.946	1.962	
C_{sat} (J K^{-1}mol^{-1})	82.96	83.69	84.52	85.44	85.74	86.41	

TABLE 46.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	21	0.845	1.90–2	0.19	–1.45–3	5
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
196.8–283.9	469.00	7.72632	3.59886	6.02818	4.14686		II



Name: Methyloxirane
Formula: C_3H_6O

CAS-RN: 75-56-9
Group No.: 46-002
Molar Mass: 58.08

TABLE 46.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
64OET		166.5–301.4	21	0.30	99.94	melpt	C_p	BSAO	58HIL/KRA
66BEA/CLE		161.3–300.0	16	nosp	99.9	melpt	C_p	BSAO	33SOU/BRI
82TAN/ZHO		170.0–325.0	32S	0.20	99.9	anal	C_{sat}	BSAO	83TAN/ZHO

52CUR/JOH technical product, purity in question

TABLE 46.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
64OET	166.5–301.4	21	0.30	0.403	1.66–2	0.12	–2.22–3	0
82TAN/ZHO	300.0–325.0	6	0.90#	0.655	8.72–2	0.59	7.23–2	4
				Rejected data				
52CUR/JOH	(5.10–1, 3.42, 5.10–1, 1)			66BEA/CLE	(4.62–1, 3.26, 4.60–1, 15)			

TABLE 46.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	70	27	0.510	4.73–2	0.32	1.43–2	4
C_{sat}	70	27	0.510	4.73–2	0.32	1.43–2	3

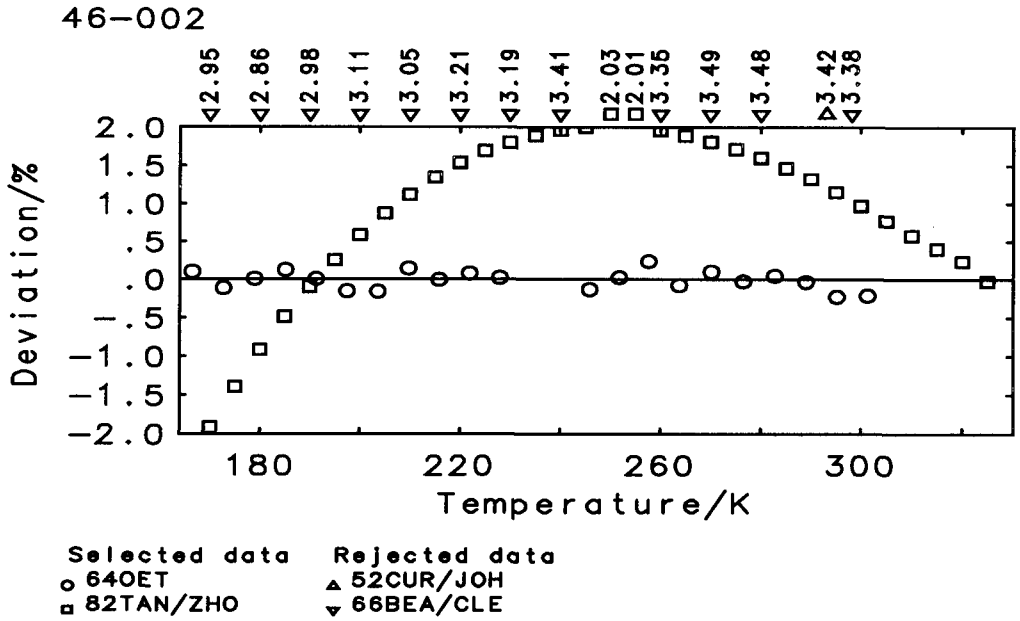
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
166.5–325.0	1.90237+1	–6.67536	2.14162	–1.37469–1	II
166.5–325.0	1.91860+1	–6.90732	2.25060	–1.54301–1	II

TABLE 46.2.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.888	1.882	1.879	1.881	1.886	1.895	1.908
C_p (J K^{-1}mol^{-1})	109.7	109.3	109.2	109.3	109.6	110.1	110.8
c_{sat} (J K^{-1}g^{-1})	1.888	1.882	1.879	1.881	1.886	1.895	1.908
C_{sat} (J K^{-1}mol^{-1})	109.7	109.3	109.2	109.2	109.6	110.1	110.8
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.924	1.943	1.965	1.991	1.999	2.019	2.050
C_p (J K^{-1}mol^{-1})	111.7	112.8	114.1	115.6	116.1	117.3	119.1
c_{sat} (J K^{-1}g^{-1})	1.924	1.943	1.965	1.991	1.999	2.019	2.050
C_{sat} (J K^{-1}mol^{-1})	111.7	112.9	114.2	115.6	116.1	117.3	119.1
Temp. (K)	298.15	300	310	320	330		
c_p (J K^{-1}g^{-1})	2.078	2.084	2.121	2.160	2.201		
C_p (J K^{-1}mol^{-1})	120.7	121.1	123.2	125.5	127.9		
c_{sat} (J K^{-1}g^{-1})	2.077	2.083	2.119	2.158	2.198		
C_{sat} (J K^{-1}mol^{-1})	120.6	121.0	123.1	125.3	127.7		

TABLE 46.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	70	22	0.770	7.28–2	0.49	–1.59–2	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
197.5–325.0	482.20	6.16873	3.92710	8.68950	2.42247		III



Name: Oxetane
Formula: C_3H_6O

CAS–RN: 503–30–0
Group No.: 46–003
Molar Mass: 58.08

TABLE 46.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
85HAN	185.0–195.0	2	1.00	100.0	chrom	C_p	BDCT	84HAN/HAW

TABLE 46.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
76CON/GIA	298.1	1	1.00#	0.000	0.00	0.00	0.00	0

TABLE 46.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		1.19766+1					V

TABLE 46.3.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	1.71
C_p (J K^{-1}mol^{-1})	99.6

Name: 1,3–Dioxolane
Formula: $C_3H_6O_2$

CAS–RN: 646–06–0
Group No.: 46–004
Molar Mass: 74.08

TABLE 46.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
69CLE/MEL4	175.9–300.0	16S	nosp	99.93	melpt	C_{sat}	BSAO	68CLE/MEL
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
88ING	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 46.4.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69CLE/MEL4	175.9–300.0	16	1.00#	0.020	2.71–3	0.02	–6.87–4	–3
76CON/GIA	298.1	1	1.00#	0.078	1.10–2	0.08	1.10–2	1
				Rejected data				
88ING	(3.54–1, 2.43, 3.54–1, 1)							

TABLE 46.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	18	17	0.029	3.99–3	0.03	2.86–6	–2
Temp. range K		A_1	A_2				Level of uncertainty
175.9–300.0		1.16659+1	8.43133–1				IV

TABLE 46.4.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c ($J K^{-1}g^{-1}$)	1.480	1.489	1.499	1.508	1.518	1.527	1.536
C ($J K^{-1}mol^{-1}$)	109.6	110.3	111.0	111.7	112.4	113.1	113.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c ($J K^{-1}g^{-1}$)	1.546	1.555	1.565	1.568	1.574	1.584	1.591
C ($J K^{-1}mol^{-1}$)	114.5	115.2	115.9	116.1	116.6	117.3	117.9
Temp. (K)	300						
c ($J K^{-1}g^{-1}$)	1.593						
C ($J K^{-1}mol^{-1}$)	118.0						

TABLE 46.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	18	17	0.028	3.87–3	0.03	–7.29–7	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
175.9–300.0	552.00	–1.76664–1	1.80069–3	1.16998+1	4.33308		IV

Name: 1,3,5-Trioxane
Formula: $C_3H_6O_3$

CAS-RN: 110–88–3
Group No.: 46–005
Molar Mass: 90.08

TABLE 46.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88VAN/VAN	337.0–346.6	7	0.15	99.95	melpt	C_p	BSAO	87VAN/VAN

TABLE 46.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	1.717	4.83–2	0.26	1.77–4	1
Temp. range K		A_1	A_2				Level of uncertainty
337.0–346.6		2.32107	4.84213				III

TABLE 46.5.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p ($J K^{-1}g^{-1}$)	1.734	1.779
C_p ($J K^{-1}mol^{-1}$)	156.2	160.2

Name: Furan
Formula: C_4H_4O

CAS–RN: 110–00–9
Group No.: 46–006
Molar Mass: 68.08

TABLE 46.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52GUT/SCO	191.0–299.1	23	0.20	99.98	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 46.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.145	3.73–3	0.03	1.33–6	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
191.0–299.1	1.74711+1	–7.20090	2.75684	–2.53697–1			II

TABLE 46.6.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.466	1.474	1.485	1.499	1.515	1.534	1.555
C_{sat} (J K^{-1}mol^{-1})	99.79	100.3	101.1	102.0	103.1	104.4	105.9
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.579	1.604	1.612	1.631	1.659	1.684	1.689
C_{sat} (J K^{-1}mol^{-1})	107.5	109.2	109.8	111.0	113.0	114.6	115.0

TABLE 46.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.742	1.88–2	0.15	4.54–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
191.0–299.1	490.20	2.40534	3.06362	7.95917	4.72125–1		II

Name: 2,3–Dihydrofuran
Formula: C_4H_6O

CAS–RN: 1191–99–7
Group No.: 46–007
Molar Mass: 70.09

TABLE 46.7.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI3	298.15	1.744	1.00	99.95	chrom	C_p	BDHT	89KNI/ARC

Name: Ethyloxirane
Formula: C_4H_8O

CAS–RN: 106–88–7
Group No.: 46–008
Molar Mass: 72.11

TABLE 46.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73GOO/FIN	136.8–322.5	24	0.20	99.93	melpt	C_{sat}	BSAO	47HUF

TABLE 46.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	1.236	3.98–2	0.25	1.60–4	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
136.8–322.5		2.14678+1	–6.83560	2.38554	–1.74270–1		II

TABLE 46.8.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J $K^{-1}g^{-1}$)	1.856	1.844	1.836	1.832	1.831	1.833	1.839
C_{sat} (J $K^{-1}mol^{-1}$)	133.8	133.0	132.4	132.1	132.0	132.2	132.6
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J $K^{-1}g^{-1}$)	1.847	1.859	1.873	1.890	1.910	1.932	1.957
C_{sat} (J $K^{-1}mol^{-1}$)	133.2	134.0	135.1	136.3	137.7	139.3	141.1
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J $K^{-1}g^{-1}$)	1.965	1.984	2.013	2.038	2.044	2.077	2.111
C_{sat} (J $K^{-1}mol^{-1}$)	141.7	143.1	145.1	147.0	147.4	149.8	152.2

TABLE 46.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	18	1.675	5.59–2	0.33	2.91–4	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
175.7–322.5	525.40	9.35012	6.26877	8.99120	3.48651	III

Name: Tetrahydrofuran
Formula: C_4H_8O

CAS-RN: 109-99-9
Group No.: 46-009
Molar Mass: 72.11

TABLE 46.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76BON/CER		298.1	1	nosp	not specified		C_p	BSIO	76BON/CER
76CON/GIA		298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
78LEB/RAB	N	161.6–322.6	50	0.20	99.8	melpt	C_p	BSAO	76LEB/LIT
79KIY/DAR		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
85COS/PAT9		283.1–313.1	3	nosp	99.5	chrom	C_p	FSIT	71PIC/LED
88ING		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED

78LEB/RAB same data in 79LEB/LIT

TABLE 46.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
78LEB/RAB	161.6–322.6	50	0.20	0.553	1.59–2	0.11	4.79–5	–4
85COS/PAT9	283.1–313.1	3	0.50#	0.057	4.12–3	0.03	–1.16–3	0
				Rejected data				
76BON/CER	(4.91–1, 3.40,–4.91–1, –1)			76CON/GIA	(4.31–1, 2.97, –4.31–1, –1)			
79KIY/DAR	(6.28–2, 0.42,–6.28–2, –1)			88ING	(1.40–1, 0.95,–1.40–1, –1)			

TABLE 46.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	57	53	0.559	1.61–2	0.11	–2.06–5	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
161.6–322.6		2.10124+1	–1.01000+1	3.67778	–3.27071–1		II

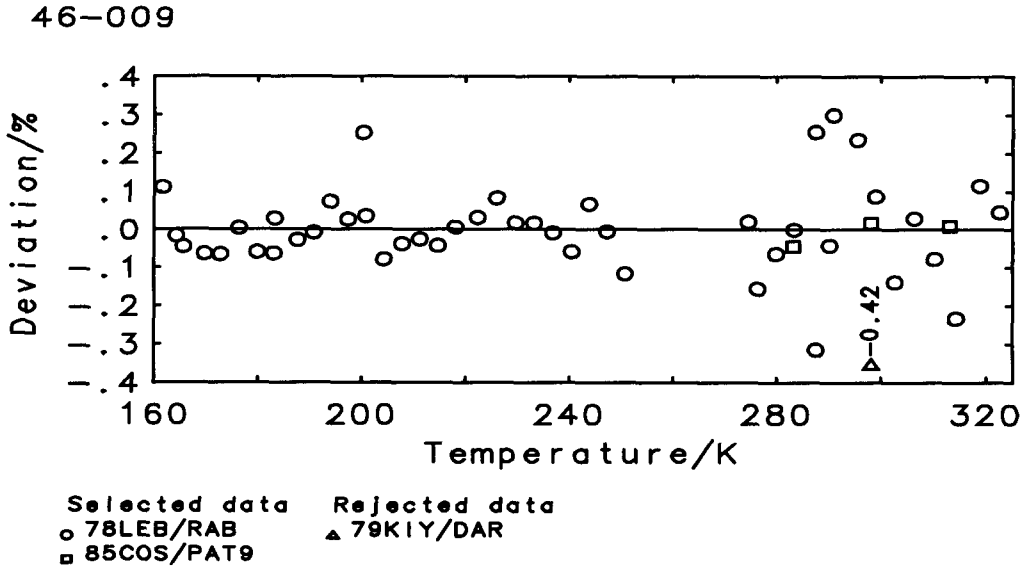
TABLE 46.9.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.483	1.481	1.482	1.488	1.498	1.512	1.529
C_p (J K^{-1}mol^{-1})	107.0	106.8	106.9	107.3	108.0	109.0	110.2
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.549	1.573	1.599	1.628	1.637	1.659	1.692
C_p (J K^{-1}mol^{-1})	111.7	113.4	115.3	117.4	118.1	119.6	122.0
Temp. (K)	298.15	300	310	320			
c_p (J K^{-1}g^{-1})	1.721	1.727	1.764	1.803			
C_p (J K^{-1}mol^{-1})	124.1	124.6	127.2	130.0			

TABLE 46.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	57	41	0.662	1.93–2	0.13	9.01–4	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
183.0–322.6	540.10	4.21525+2	3.97814+1	–3.11126+1	4.29479+2	–2.04719+1	3.85735+2	II



Name: 1,3–Dioxane
Formula: $C_4H_8O_2$

CAS–RN: 505–22–6
Group No.: 46–010
Molar Mass: 88.11

TABLE 46.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
88ING	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 46.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76CON/GIA	298.1	1	1.00#	1.254	2.17–1	1.25	–2.17–1	–1
88ING	298.1	1	0.50#	0.637	5.60–2	0.32	5.60–2	1

TABLE 46.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	1.406	2.24–1	1.29	–8.05–2	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		1.75277+1					IV

TABLE 46.10.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	1.654
C_p (J K^{-1}mol^{-1})	145.7

Name: 1,4–Dioxane
Formula: $C_4H_8O_2$

CAS–RN: 123–91–1
Group No.: 46–011
Molar Mass: 88.11

TABLE 46.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
29HER/LOR	296.1	1	nosp	not specified		C_p	DSIO	22HER/SCH
33ROT/MEY1	291.1	1	nosp	not specified		C_p	DSIO	33ROT/MEY2
34JAC/PAR	288.7–298.2	3	nosp	not specified		C_p	BSIO	25PAR
52STA/AMI	313.1	1	nosp	not specified		C_p	BSIO	52STA/AMI
61ROU	296.9–313.7	14	nosp	not specified		C_p	BSAO	61ROU
71DES/BHA	298.1–318.1	3S	nosp	not specified		C_p	BSIO	56MUR/VAN
71KHA/SUB	298.1–313.1	2	nosp	not specified		C_p	BSIO	64MOE/THO
76BON/CER	298.1	1	nosp	not specified		C_p	BSIO	76BON/CER
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
79MUR/SUB	298.1	1	nosp	not specified		C_p	BSIO	64MOE/THO
84GRO/ING	298.1	1	0.30	99.5	melpt	C_p	FSIT	71PIC/LED
84ING/GRO	298.1	1	0.30	99.5	chrom	C_p	FSIT	71PIC/LED
88ING	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
89BAR/KOO2	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
91GRO/ROU	298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
91TRE/COS	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 46.11.2. Correlated heat capacities

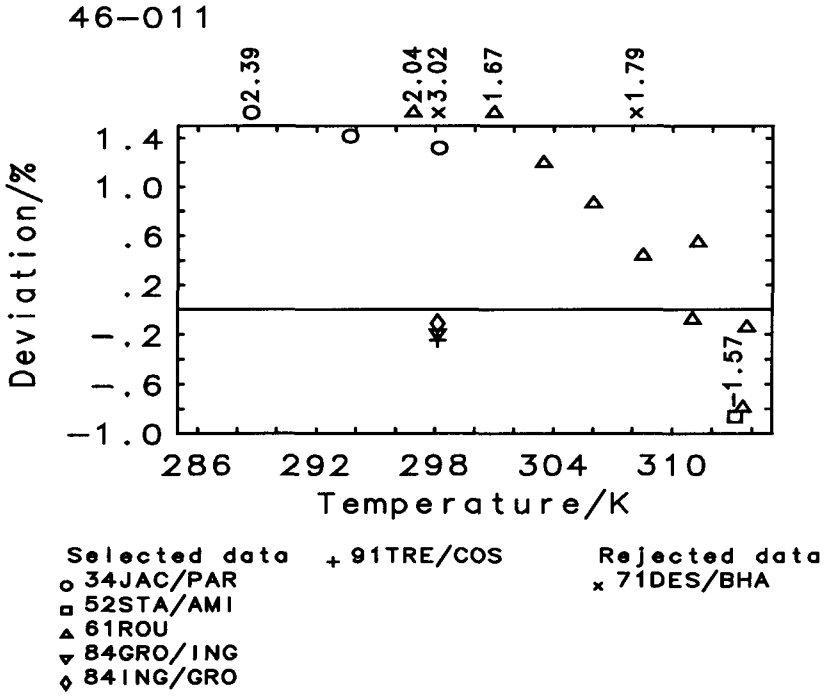
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
34JAC/PAR	288.7–298.2	3	1.00#	1.776	3.23–1	1.78	3.11–1	3
52STA/AMI	313.1	1	2.00#	0.788	2.94–1	1.58	–2.94–1	–1
61ROU	296.9–313.7	14	1.00#	1.152	2.14–1	1.15	1.55–1	8
76BON/CER	298.1	1	1.50#	0.871	2.34–1	1.31	–2.34–1	–1
79MUR/SUB	298.1	1	2.00#	0.653	2.34–1	1.31	–2.34–1	–1
84GRO/ING	298.1	1	0.30	0.655	3.56–2	0.20	–3.56–2	–1
84ING/GRO	298.1	1	0.30	0.389	2.12–2	0.12	–2.12–2	–1
88ING	298.1	1	0.50#	1.624	1.46–1	0.81	–1.46–1	–1
89BAR/KOO2	298.1	1	0.50#	1.948	1.75–1	0.97	–1.75–1	–1
91GRO/ROU	298.1	1	0.50#	1.719	1.55–1	0.86	–1.55–1	–1
91TRE/COS	298.1	1	0.50#	0.500	4.52–2	0.25	–4.52–2	–1
				Rejected data				
29HER/LOR	(5.72–1, 3.07, 5.72–1, 1)			33ROT/MEY1	(6.14–1, 3.34, 6.14–1, 1)			
71DES/BHA	(4.67–1, 2.48, 4.53–1, 2)			71KHA/SUB	(4.15–1, 2.28, –4.12–1, –2)			
76CON/GIA	(1.30, 7.69,–1.30, –1)							

TABLE 46.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	26	1.292	2.26–1	1.23	6.76–2	2
Temp. range K		A_1	A_2				Level of uncertainty
288.7–313.7		2.45757	5.26479				V

TABLE 46.11.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.67	1.71	1.72	1.77
C_p (J K^{-1}mol^{-1})	147	151	152	156



Name: 1,3,5,7-Tetroxocane
Formula: $C_4H_8O_4$

CAS-RN: 293-30-1
Group No.: 46-012
Molar Mass: 120.11

TABLE 46.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69CLE/MEL1	395.0–420.0	14S	2.00	not specified		C_p	BDHT	69PER/COM

TABLE 46.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	14	14	0.283	1.67-1	0.57	1.51-3	-6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
395.0–420.0		4.26418+2	-1.97624+2	2.45538+1			V

TABLE 46.12.4. Recommended values of heat capacities

Temp. (K)	400	410	420
c_p (J K^{-1}g^{-1})	1.99	2.00	2.04
C_p (J K^{-1}mol^{-1})	239	240	245

Name: 2–Methylfuran
Formula: C_5H_6O

CAS–RN: 534–22–5
Group No.: 46–013
Molar Mass: 82.10

TABLE 46.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65CAR/WES1	196.3–306.9	13	0.50	99.16	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 46.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	13	13	0.073	6.08–3	0.04	4.18–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
196.3–306.9		2.28415+1	–9.18089	3.40927	–3.20276–1		III

TABLE 46.13.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J $K^{-1}g^{-1}$)	1.575	1.583	1.593	1.607	1.622	1.640	1.660
C_{sat} (J $K^{-1}mol^{-1}$)	129.3	130.0	130.8	131.9	133.2	134.6	136.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J $K^{-1}g^{-1}$)	1.681	1.689	1.705	1.729	1.751	1.756	1.783
C_{sat} (J $K^{-1}mol^{-1}$)	138.0	138.6	140.0	142.0	143.7	144.1	146.4

TABLE 46.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	13	13	0.325	2.63–2	0.16	6.25–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
196.3–306.9	527.00	6.41110	5.32620	9.27529	1.92925		III

Name: Tetrahydropyran
Formula: $C_5H_{10}O$

CAS–RN: 142–68–7
Group No.: 46–014
Molar Mass: 86.13

TABLE 46.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64MOE/THO	297.6–327.5	4S	0.50	not specified		C_p	BSIO	64MOE/THO
76CON/GIA	298.1	1	nosp	not specified		C_p	BDCT	76CON/GIA
84ING/GRO	298.1	1	0.30	99.	chrom	C_p	FSIT	71PIC/LED
88ING	298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

TABLE 46.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64MOE/THO	297.6–327.5	4	0.50	1.097	1.01–1	0.55	6.00–2	2
84ING/GRO	298.1	1	0.30	0.918	4.95–2	0.28	–4.95–2	–1
88ING	298.1	1	0.50#	1.075	9.64–2	0.54	–9.64–2	–1
				Rejected data				
76CON/GIA	(1.13, 6.71,–1.13, –1)							

TABLE 46.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	1.305	1.15–1	0.63	1.57–2	0
Temp. range K		A_1	A_2				Level of uncertainty
297.6–327.5		3.32583	4.93588				IV

TABLE 46.14.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p (J K^{-1}g^{-1})	1.750	1.798	1.846	1.893
C_p (J K^{-1}mol^{-1})	150.8	154.9	159.0	163.1

Name: 1,3–Dioxepane
Formula: $C_5H_{10}O_2$

CAS–RN: 505–65–7
Group No.: 46–015
Molar Mass: 102.13

TABLE 46.15.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76CON/GIA	298.15	1.639	nosp	not specified		C_p	BDCT	76CON/GIA

Name: 1,3,5,7,9–Pentoxecane
Formula: $C_5H_{10}O_5$

CAS–RN: 16528–92–0
Group No.: 46–016
Molar Mass: 150.13

TABLE 46.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
69CLE/MEL3	334.0–390.0	7S	2.00	not specified		C_{sat}	BDHT	69PER/COM

TABLE 46.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.009	5.58–3	0.02	2.18–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
334.0–390.0		2.17482+1	2.64757				V

TABLE 46.16.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390
c_{sat} (J K^{-1}g^{-1})	1.70	1.72	1.73	1.75	1.76	1.78
C_{sat} (J K^{-1}mol^{-1})	256	258	260	262	264	267

Name: 7–Oxabicyclo[4.1.0]heptane
Formula: $C_6H_{10}O$

CAS–RN: 286–20–4
Group No.: 46–017
Molar Mass: 98.14

TABLE 46.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80NAK/SUG	239.0–297.0	24	0.30	99.973	melpt	C_{sat}	BSAO	65SUG/SEK

TABLE 46.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	23	0.137	7.89–3	0.04	2.41–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
240.4–297.0		3.40707+1	–2.33769+1	9.59784	–1.12424		II

TABLE 46.17.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.500	1.529	1.560	1.592	1.602	1.625	1.658
C_{sat} (J K^{-1}mol^{-1})	147.2	150.1	153.1	156.3	157.3	159.5	162.8
Temp. (K)	298.15	300					
c_{sat} (J K^{-1}g^{-1})	1.685	1.691					
C_{sat} (J K^{-1}mol^{-1})	165.4	166.0					

Name: 2,4,6–Trimethyl–1,3,5–trioxane
Formula: $C_6H_{12}O_3$

CAS–RN: 123–63–7
Group No.: 46–018
Molar Mass: 132.16

TABLE 46.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON	306.6–345.6	4S	nosp	not specified	C_{avg}	DSIO	*81VON
39PHI	306.5	1	nosp	not specified	C_p	BSIO	49WEI
69CLE/MEL2	287.5–315.8	10	1.00	not specified	C_p	BSAO	68CLE/MEL

TABLE 46.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69CLE/MEL2	287.5–315.8	10	1.00	0.382	1.18–1	0.38	8.97–4	1
				Rejected data				
*81VON	(2.23, 7.67,–2.23, –1)			39PHI	(8.00–1, 2.62,–8.00–1, –1)			

TABLE 46.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	10	0.428	1.32–1	0.43	8.97–4	1
Temp. range K		A_1	A_2				Level of uncertainty
287.5–315.8		1.82614+1	4.26167				V

TABLE 46.18.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.93	1.95	1.95	1.98	2.01
C_p (J K^{-1}mol^{-1})	255	257	258	262	265

Name: Benzofuran
Formula: C_8H_6O

CAS–RN: 271–89–6
Group No.: 46–019
Molar Mass: 118.14

TABLE 46.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
65ZIE	N	315.6–369.0	3	nosp	not specified	C_{avg}	DSIO	58SWI/ZIE1
86CHI/NGU		245.5–450.0	24S	0.07	99.977 melpt	C_{sat}	BSAO	47HUF

65ZIE average values in temperature ranges 295–443 K, 294–373 K and 294–338 K

TABLE 46.19.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
86CHI/NGU	245.5–450.0	24	0.07	0.242	3.80–3	0.02	1.03–6	–1
				Rejected data				
65ZIE	(2.49–1, 1.09,–2.44–1, –3)							

TABLE 46.19.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	24	0.272	4.28–3	0.02	1.03–6	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
245.5–335.0	2.53286+1	–9.35686	3.77285	–3.57418–1			II
335.0–450.0	1.52985+1	–3.74610–1	1.09158	–9.06246–2			II

TABLE 46.19.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.403	1.423	1.445	1.452	1.468	1.493	1.513
C_{sat} (J K^{-1}mol^{-1})	165.7	168.1	170.7	171.6	173.5	176.3	178.7
Temp. (K)	300	310	320	330	340	350	360
c_{sat} (J K^{-1}g^{-1})	1.518	1.544	1.570	1.597	1.625	1.652	1.680
C_{sat} (J K^{-1}mol^{-1})	179.3	182.4	185.5	188.7	191.9	195.2	198.5
Temp. (K)	370	380	390	400	410	420	430
c_{sat} (J K^{-1}g^{-1})	1.708	1.736	1.764	1.792	1.820	1.849	1.877
C_{sat} (J K^{-1}mol^{-1})	201.8	205.1	208.4	211.7	215.1	218.4	221.7
Temp. (K)	440	450					
c_{sat} (J K^{-1}g^{-1})	1.905	1.933					
C_{sat} (J K^{-1}mol^{-1})	225.0	228.3					

TABLE 46.19.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	24	3.179	5.04–2	0.22	2.21–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
245.5–450.0	679.00	–4.13190	2.66309–1	1.16490+1	1.60270+1		II

Name: 2,3–Dihydrobenzofuran
Formula: C_8H_8O

CAS–RN: 496–16–2
Group No.: 46–020
Molar Mass: 120.15

TABLE 46.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86CHI/NGU	250.9–450.0	23S	0.07	99.992	melpt	C_{sat}	BSAO	47HUF

TABLE 46.20.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.143	2.44–3	0.01	9.12–7	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
250.9–345.0	2.56695+1	–8.83994	3.62108	–3.32555–1	II
345.0–450.0	1.71713+1	–1.45023	1.47913	–1.25603–1	II

TABLE 46.20.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J $K^{-1}g^{-1}$)	1.475	1.498	1.506	1.523	1.548	1.570	1.575
C_{sat} (J $K^{-1}mol^{-1}$)	177.3	180.0	180.9	183.0	186.0	188.6	189.2
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J $K^{-1}g^{-1}$)	1.602	1.631	1.659	1.689	1.718	1.748	1.778
C_{sat} (J $K^{-1}mol^{-1}$)	192.5	195.9	199.4	202.9	206.4	210.0	213.6
Temp. (K)	380	390	400	410	420	430	440
c_{sat} (J $K^{-1}g^{-1}$)	1.808	1.838	1.868	1.898	1.928	1.958	1.988
C_{sat} (J $K^{-1}mol^{-1}$)	217.2	220.9	224.5	228.1	231.7	235.3	238.8
Temp. (K)	450						
c_{sat} (J $K^{-1}g^{-1}$)	2.017						
C_{sat} (J $K^{-1}mol^{-1}$)	242.4						

TABLE 46.20.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	2.916	4.94–2	0.20	1.97–4	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
250.9–450.0	705.00	–4.82367	3.19617–1	1.18382+1	1.81997+1	II

Name: 3–Oxabicyclo[3.2.2]nonane
Formula: $C_8H_{14}O$

CAS–RN: 283–27–2
Group No.: 46–021
Molar Mass: 126.20

TABLE 46.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70WES/WON	454.5–477.0	6	0.10	99.66	melpt	C_p	BSAO	68WES/WES

TABLE 46.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	No. data points used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	2.640	9.38–2	0.26	3.24–4	0

Temp. range K	A_1	A_2	Level of uncertainty
454.5–477.0	–1.69945	8.02134	III

TABLE 46.21.4. Recommended values of heat capacities

Temp. (K)	450	460	470	480
c_p (J $K^{-1}g^{-1}$)	2.266	2.319	2.372	2.425
C_p (J $K^{-1}mol^{-1}$)	286.0	292.7	299.3	306.0

Name: 1,4,7,10–Tetraoxacyclododecane
Formula: $C_8H_{16}O_4$

CAS–RN: 294–93–9
Group No.: 46–022
Molar Mass: 176.21

TABLE 46.22.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90BRI/WAD	298.15	1.734	nosp	99.5	anal	C_p	DDCT	74SUU/WAD

Name: 3,4–Dihydro–1*H*–2–benzopyran
Formula: $C_9H_{10}O$

CAS–RN: 493–05–0
Group No.: 46–023
Molar Mass: 134.18

TABLE 46.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90CHI/ARC	N	272.9–439.8	21	0.10	99.924	melpt	C_{sat}	BSAO	47HUF

90CHI/ARC smoothed data in 86CHI/NGU

TABLE 46.23.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.187	5.03–3	0.02	1.73–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
272.9–355.0		2.69479+1	–8.40251	3.78512	–3.52657–1		II
355.0–439.8		1.57599+1	1.05220	1.12182	–1.02581–1		II

TABLE 46.23.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.571	1.600	1.623	1.629	1.659	1.689	1.721
C_{sat} (J K^{-1}mol^{-1})	210.8	214.6	217.8	218.5	222.6	226.7	230.9
Temp. (K)	340	350	360	370	380	390	400
c_{sat} (J K^{-1}g^{-1})	1.752	1.784	1.816	1.848	1.879	1.911	1.943
C_{sat} (J K^{-1}mol^{-1})	235.1	239.3	243.6	247.9	252.2	256.4	260.7
Temp. (K)	410	420	430	440			
c_{sat} (J K^{-1}g^{-1})	1.974	2.006	2.037	2.068			
C_{sat} (J K^{-1}mol^{-1})	264.9	269.1	273.3	277.5			

TABLE 46.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.959	2.69–2	0.10	5.56–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
272.9–439.8	728.40	–3.23013	8.70464–2	1.21030+1	2.99661+1		II

Name: 3,4–Dihydro–2*H*–1–benzopyran
Formula: $C_9H_{10}O$

CAS–RN: 493–08–3
Group No.: 46–024
Molar Mass: 134.18

TABLE 46.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
90CHI/ARC	N	275.0–441.6	18	0.10	99.987	melpt	C_{sat}	BSAO	47HUF

90CHI/ARC smoothed data in 86CHI/NGU

TABLE 46.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.197	6.13–3	0.02	2.86–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
275.0–441.6		2.07464+1	–3.45496	2.34794	–2.10538–1		II

TABLE 46.24.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.511	1.520	1.540	1.570	1.595	1.600	1.631
C_{sat} (J K^{-1}mol^{-1})	202.8	204.0	206.7	210.7	214.0	214.8	218.9
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	1.663	1.695	1.727	1.759	1.792	1.824	1.857
C_{sat} (J K^{-1}mol^{-1})	223.1	227.4	231.7	236.0	240.4	244.8	249.2
Temp. (K)	390	400	410	420	430	440	
c_{sat} (J K^{-1}g^{-1})	1.890	1.922	1.954	1.986	2.018	2.049	
C_{sat} (J K^{-1}mol^{-1})	253.6	257.9	262.2	266.5	270.8	274.9	

TABLE 46.24.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.967	2.77–2	0.10	5.85–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
275.0–441.6	727.40	–2.49750	4.81945–2	1.10939+1	3.23559+1		II

Name: 1,4,7,10,13–Pentaoxacyclopentadecane
Formula: $C_{10}H_{20}O_5$

CAS–RN: 33100–27–5
Group No.: 46–025
Molar Mass: 220.27

TABLE 46.25.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
90BRI/WAD	298.15	1.783	nosp	99.5	anal	C_p	DDCT	74SUU/WAD

Name: Dibenzofuran
Formula: $C_{12}H_8O$

CAS–RN: 132–64–9
Group No.: 46–026
Molar Mass: 168.19

TABLE 46.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
90CHI/GAM	362.0–520.3	17	0.10	99.955	melpt	C_{sat}	BSAO	47HUF
90CHI/GAM	400.0–720.0	17	1.00	99.955	melpt	C_{sat}	BDHT	89KNI/ARC

TABLE 46.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
90CHI/GAM	362.0–520.3	17	0.10	0.416	1.60–2	0.04	3.66–4	3
90CHI/GAM	400.0–720.0	17	1.00	0.230	1.04–1	0.23	–3.47–2	–4

TABLE 46.26.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.364	8.08–2	0.18	–1.71–2	–1
C_{sat}	34	34	0.340	7.16–2	0.16	–1.59–2	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
362.0–520.0	1.27391+1	4.54574	3.85037–1	–4.48775–2	II
520.0–720.0	–9.40903	1.73235+1	–2.07223	1.12640–1	IV
362.0–520.0	1.30689+1	4.29352	4.48968–1	–5.02454–2	II
520.0–720.0	–2.71868	1.34018+1	–1.30262	6.20361–2	IV

TABLE 46.26.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c_p (J K^{-1}g^{-1})	1.582	1.609	1.637	1.664	1.691	1.718	1.745
C_p (J K^{-1}mol^{-1})	266.1	270.7	275.3	279.9	284.4	289.0	293.5
c_{sat} (J K^{-1}g^{-1})	1.582	1.609	1.637	1.664	1.691	1.718	1.745
C_{sat} (J K^{-1}mol^{-1})	266.1	270.7	275.3	279.9	284.4	289.0	293.5
Temp. (K)	430	440	450	460	470	480	490
c_p (J K^{-1}g^{-1})	1.772	1.798	1.824	1.850	1.876	1.902	1.927
C_p (J K^{-1}mol^{-1})	298.0	302.4	306.8	311.2	315.5	319.8	324.1
c_{sat} (J K^{-1}g^{-1})	1.772	1.798	1.824	1.850	1.876	1.901	1.927
C_{sat} (J K^{-1}mol^{-1})	298.0	302.4	306.8	311.2	315.5	319.8	324.1
Temp. (K)	500	510	520	530	540	550	560
c_p (J K^{-1}g^{-1})	1.952	1.977	2.001	2.025	2.049	2.073	2.096
C_p (J K^{-1}mol^{-1})	328.3	332.4	336.6	340.6	344.6	348.6	352.5
c_{sat} (J K^{-1}g^{-1})	1.952	1.976	2.001	2.025	2.048	2.072	2.095
C_{sat} (J K^{-1}mol^{-1})	328.3	332.4	336.5	340.5	344.5	348.4	352.3
Temp. (K)	570	580	590	600	610	620	630
c_p (J K^{-1}g^{-1})	2.119	2.142	2.165	2.188	2.211	2.234	2.257
C_p (J K^{-1}mol^{-1})	356.4	360.3	364.2	368.0	371.9	375.7	379.5
c_{sat} (J K^{-1}g^{-1})	2.118	2.140	2.163	2.185	2.207	2.229	2.250
C_{sat} (J K^{-1}mol^{-1})	356.2	360.0	363.7	367.5	371.2	374.9	378.5
Temp. (K)	640	650	660	670	680	690	700
c_p (J K^{-1}g^{-1})	2.279	2.302	2.326	2.349	2.372	2.396	2.420
C_p (J K^{-1}mol^{-1})	383.4	387.3	391.1	395.1	399.0	403.0	407.0
c_{sat} (J K^{-1}g^{-1})	2.272	2.293	2.315	2.336	2.357	2.379	2.400
C_{sat} (J K^{-1}mol^{-1})	382.1	385.7	389.3	392.9	396.5	400.1	403.6
Temp. (K)	710	720					
c_p (J K^{-1}g^{-1})	2.444	2.469					
C_p (J K^{-1}mol^{-1})	411.1	415.2					
c_{sat} (J K^{-1}g^{-1})	2.421	2.442					
C_{sat} (J K^{-1}mol^{-1})	407.2	410.7					

TABLE 46.26.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.799	2.13–1	0.46	–4.83–2	–7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
362.0–720.0	824.00	4.07842	7.89765–2	1.11973+1	5.26534+1		III

47. Miscellaneous Oxygen Compounds

The miscellaneous oxygen family consists of 51 compounds containing two and more oxygen atoms which could not be included in any of the preceding oxygen families. A total of 12 compounds of this family were measured at one temperature only. For one of the compounds, only the table of experimental values is given for trimellitic anhydride as measured at RAB (78MAR/CIO2). These data seems to be wrong as are all other data from this laboratory.

Most compounds from this family were investigated at CIUG (78KAR/LEB, 78KAR/RAB, 80KUL/LEB, 81LEB/EVS1, 83LEB/EVS, 83LEB/KUL, 86RAB/SHE) where attention was paid mainly to substances used in macromolecular chemistry. The reported error of around 0.3 % seems to be realistic with the exception of 1,4-dioxane-2,5-dione (88LEB/KUL) where the reported uncertainty is larger (1 %). Data are reported for γ-butyrolactone from CIUG data (83LEB/EVS); also, one data point at 298.15 K is reported from NIPER (89STE/CHI3). The latter value differs, however, from the former values by almost 50 % and is obviously in error. Four homologues of oxo-diols (from di- to pentaethyleneglycols) were measured at UCCW (79STE/TAM) where examination of the data by us resulted in an uncertainty estimate of 1 %. A similar examination for measurements from LSU (73VAS/KOR, 76VAS/KOR) was made for two cyclic miscellaneous oxygen compounds yielding an estimated uncertainty of 1 %. Two cyclic compounds (87LES/LIS) were studied at IURP (87LES/LIS) using a DSC instrument and the measured C_p values exhibited a linear variation with temperature; a reported error of 2 % was given. However, the authors surprisingly fit the data to a third degree polynomial. Three 2-alkyloxyethanols were measured at ICTP (91SVO/ZAB2) and the results showed an error below 0.5 %.

Nearly no parallel measurements from different laboratories were performed for most of compounds. The data for furfural are an exception where the GPI values (67RAS/GAN) were selected from measurements of several laboratories for establishing the recommended values. The data for furfuryl alcohol is another exception where recommended values are based on SUC values (56PAR/KEN) supplemented by values from CITP (50HOU/MAS2).

Measurements were made on some high molar mass glyceryl esters, 1-monostearin and 3-aceto-1-stearin (55WAR/VIC), and on compounds belonging to the class of liquid crystals (74AND/BAC, 83ANI/VOR, 85SHA/ZHU).

Name: 2–Oxetanone
Formula: $C_3H_4O_2$

CAS–RN: 57–57–8
Group No.: 47–001
Molar Mass: 72.06

TABLE 47.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83LEB/EVS	N	244.1–340.9	25	0.30	99.05	melpt	C_p	BSAO	76LEB/LIT

83LEB/EVS smoothed values in 79EVS/LEB2

TABLE 47.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	0.680	3.00–2	0.20	1.07–4	–5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
244.1–340.9		1.44820+1	–1.39751	4.86865–1			III

TABLE 47.1.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1}g^{-1}$)	1.619	1.631	1.645	1.650	1.660	1.676	1.689
C_p ($J K^{-1}mol^{-1}$)	116.7	117.6	118.5	118.9	119.6	120.8	121.8
Temp. (K)	300	310	320	330	340		
c_p ($J K^{-1}g^{-1}$)	1.693	1.711	1.730	1.751	1.772		
C_p ($J K^{-1}mol^{-1}$)	122.0	123.3	124.7	126.1	127.7		

TABLE 47.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	0.687	3.03–2	0.21	1.09–4	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
244.1–340.9	675.00	3.80376	5.02004	7.54969	7.20541–1		III

Name: 1,3–Dioxolan–2–one
Formula: $C_3H_4O_3$

CAS–RN: 96–49–1
Group No.: 47–002
Molar Mass: 88.06

TABLE 47.2.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
58PEP		323.1	1	nosp	not specified		C_p	not specified	
73VAS/KOR	N	309.5–350.0	5S	nosp	99.83	melpt	C_p	BSAO	77KU/COM

73VAS/KOR selected data in 74VAS/KOR and 75VAS/VAS

TABLE 47.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73VAS/KOR	309.5–350.0	5	1.00#	0.000	4.18–6	0.00	0.00	0
				Rejected data				
58PEP	(7.80–1, 4.85,–7.80–1, –1)							

TABLE 47.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	5	0.000	5.39–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
309.5–350.0		1.07020+1	1.90754				IV

TABLE 47.2.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.569	1.587	1.605	1.623	1.641
C_p ($J K^{-1} mol^{-1}$)	138.1	139.7	141.3	142.9	144.5

Name: (*R*,*S*)–2–Hydroxypropanoic acid
Formula: $C_3H_6O_3$

CAS–RN: 598–82–3
Group No.: 47–003
Molar Mass: 90.08

TABLE 47.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36PAR/THO	290.0–300.0	2S	1.00	97.	anal	C_p	BSIO	25PAR

TABLE 47.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
290.0–300.0	1.32815+1	4.07961	IV

TABLE 47.3.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	2.318	2.349	2.356
C_p ($J K^{-1} mol^{-1}$)	208.8	211.6	212.2

Name: 2–Methoxyethanol
Formula: $C_3H_8O_2$

CAS–RN: 109–86–4
Group No.: 47–004
Molar Mass: 76.10

TABLE 47.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
73KUS/SUU		298.1	1	nosp	not specified		C_p	DDCT	71KON/SUU
78ROU/PER2		298.1	1	nosp	99.	chrom	C_p	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
91SVO/ZAB2		300.6–328.3	7	0.50	99.95	chrom	C_p	BSAO	91SVO/ZAB1
93PAG/HUO		298.1–313.1	2	nosp	99.7	anal	C_p	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question

TABLE 47.4.2. Correlated heat capacities

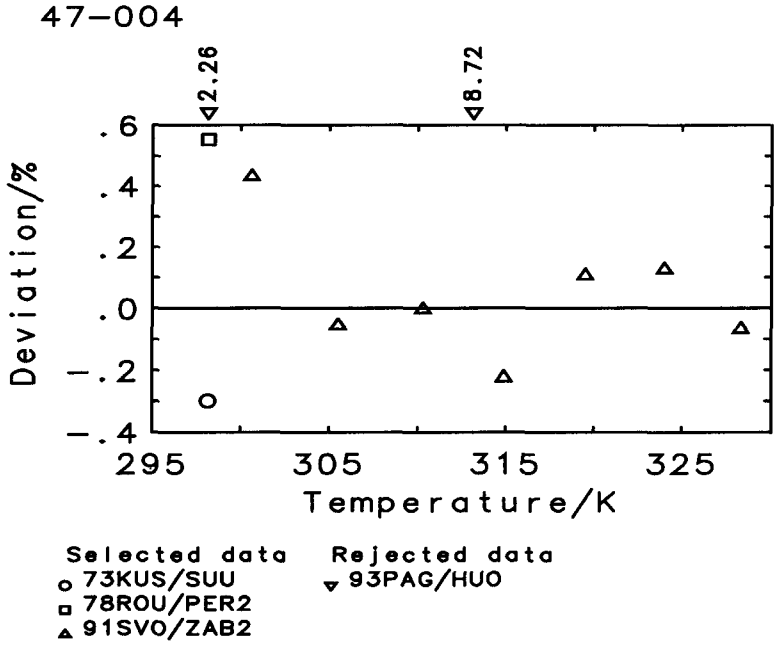
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KUS/SUU	298.1	1	0.30#	1.004	6.34–2	0.30	–6.34–2	–1
78ROU/PER2	298.1	1	0.50#	1.103	1.17–1	0.55	1.17–1	1
91SVO/ZAB2	300.6–328.3	7	0.50	0.393	4.21–2	0.20	8.94–3	0
				Rejected data				
89COB/GAR	(3.61–1, 1.74,–3.61–1, –1)			93PAG/HUO	(1.50, 6.37, 1.27, 2)			

TABLE 47.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	9	0.742	7.08–2	0.33	1.29–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.1–328.3		3.35448+1	–1.14047+1	2.42508			III

TABLE 47.4.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.280	2.305	2.312	2.349	2.391	2.439
C_p (J K^{-1}mol^{-1})	173.5	175.4	175.9	178.7	181.9	185.6



Name: 1,4–Dioxane–2,5–dione
Formula: $C_4H_4O_4$

CAS–RN: 502–97–6
Group No.: 47–005
Molar Mass: 116.07

TABLE 47.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78EVS/BEL	N	356.2–400.0	6S	0.70	99.9	chrom	C_p	BSAO	68LEA
88LEB/KUL		367.3–397.5	4	0.70	99.9	melpt	C_p	BSAO	76LEB/LIT

78EVS/BEL same data in 78LEB/EVS

TABLE 47.5.2. Correlated heat capacities

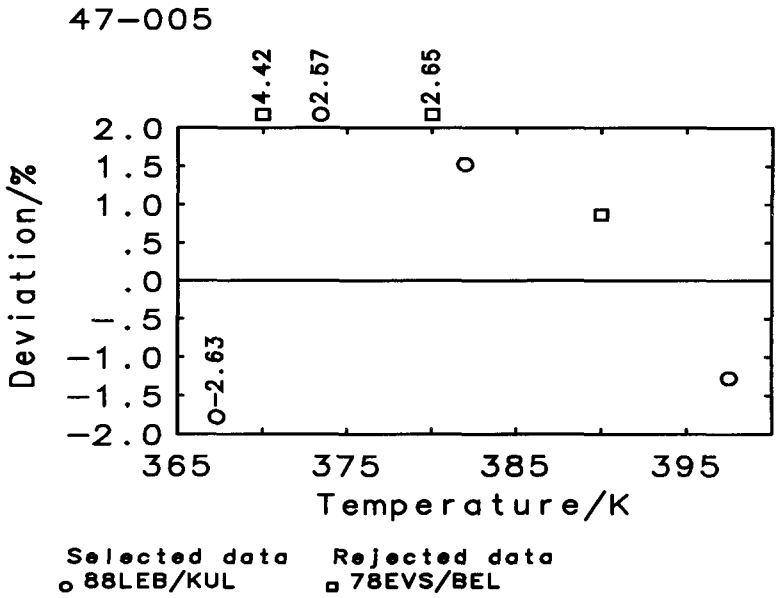
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88LEB/KUL	367.3–397.5	4	0.70	2.985	4.92–1	2.09	2.02–2	0
				Rejected data				
78EVS/BEL	(7.35–1, 3.01, 6.45–1, 3)							

TABLE 47.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	4	4.221	6.96–1	2.95	2.02–2	0
Temp. range K		A_1	A_2				Level of uncertainty
367.3–397.5		–4.65718–1	6.40520				V

TABLE 47.5.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400
c_p ($J\,K^{-1}g^{-1}$)	1.66	1.71	1.76	1.80
C_p ($J\,K^{-1}mol^{-1}$)	193	199	204	209



Name: 2(3*H*)–Dihydrofuranone
Formula: $C_4H_6O_2$

CAS–RN: 96–48–0
Group No.: 47–006
Molar Mass: 86.09

TABLE 47.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79FUC		298.1	1	0.50	99.	chrom	C_p	BSIO	80FUC
83LEB/EVS	N	232.5–328.6	28	0.30	99.83	melpt	C_p	BSAO	76LEB/LIT
89STE/CHI3		298.1	1	1.00	99.98	chrom	C_p	BDHT	89KNI/ARC

83LEB/EVS same data in 79EVS/LEB1

TABLE 47.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79FUC	298.1	1	0.50	0.124	1.05–2	0.06	1.05–2	1
83LEB/EVS	232.5–328.6	28	0.30	0.420	2.12–2	0.13	–8.10–5	–4
				Rejected data				
89STE/CHI3	(1.68+1, 49.72, 1.68+1, 1)							

TABLE 47.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	30	29	0.436	2.21–2	0.13	2.85–4	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
232.5–328.6		1.60942+1	–1.75577	6.90326–1			II

TABLE 47.6.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.517	1.531	1.547	1.564	1.583	1.589	1.602
C_p (J K^{-1}mol^{-1})	130.6	131.8	133.2	134.7	136.2	136.8	137.9
Temp. (K)	290	298.15	300	310	320	330	
c_p (J K^{-1}g^{-1})	1.623	1.641	1.646	1.669	1.694	1.721	
C_p (J K^{-1}mol^{-1})	139.8	141.3	141.7	143.7	145.9	148.1	

TABLE 47.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	30	29	0.437	2.22–2	0.13	1.70–4	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
232.5–328.6	730.00	1.28660+1	1.24486+1	1.34606	3.32437		II

Name: 4–Methyl–1,3–dioxolan–2–one
Formula: $C_4H_6O_3$

CAS–RN: 108–32–7
Group No.: 47–007
Molar Mass: 102.09

TABLE 47.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
58PEP		323.1	1	nosp	not specified		C_p	not specified	
76VAS/KOR	N	226.7–416.3	93	nosp	99.32	melpt	C_p	BSAO	77KU/COM
91WIL/JIM		298.1	1	nosp	99.	anal	C_p	FSIT	71PIC/LED

76VAS/KOR smoothed data in 74VAS/KOR

TABLE 47.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76VAS/KOR	226.7–416.3	93	1.00#	0.559	1.19–1	0.56	2.58–2	20
91WIL/JIM	298.1	1	0.50#	5.516	5.38–1	2.76	–5.38–1	–1
				Rejected data				
58PEP	(1.45, 6.56, 1.45, 1)							

TABLE 47.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	95	94	0.813	1.34–1	0.64	1.98–2	19
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
226.7–416.3		3.25055+1	−1.45587+1	4.78626	−4.37136−1		IV

TABLE 47.7.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.549	1.555	1.563	1.574	1.587	1.591	1.602
C_p (J K^{-1}mol^{-1})	158.2	158.7	159.6	160.7	162.0	162.5	163.5
Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.619	1.634	1.637	1.657	1.678	1.700	1.723
C_p (J K^{-1}mol^{-1})	165.3	166.8	167.1	169.2	171.3	173.6	175.9
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	1.746	1.770	1.793	1.817	1.840	1.863	1.885
C_p (J K^{-1}mol^{-1})	178.3	180.7	183.1	185.5	187.9	190.2	192.4
Temp. (K)	420						
c_p (J K^{-1}g^{-1})	1.906						
C_p (J K^{-1}mol^{-1})	194.6						

TABLE 47.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	95	94	0.897	1.40–1	0.67	−1.92–3	15
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
226.7–416.3	779.00	1.91178	7.40187	9.04091	1.23445–1		IV

Name: 2–Ethoxyethanol
Formula: $C_4H_{10}O_2$

CAS–RN: 110–80–5
Group No.: 47–008
Molar Mass: 90.12

TABLE 47.8.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
73KUS/SUU		298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
78ROU/PER2		283.1–313.1	3	nosp	99.	chrom	C_p	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
91SVO/ZAB2		300.6–328.3	7	0.50	99.95	chrom	C_p	BSAO	91SVO/ZAB1

52CUR/JOH technical product, purity in question

TABLE 47.8.2. Correlated heat capacities

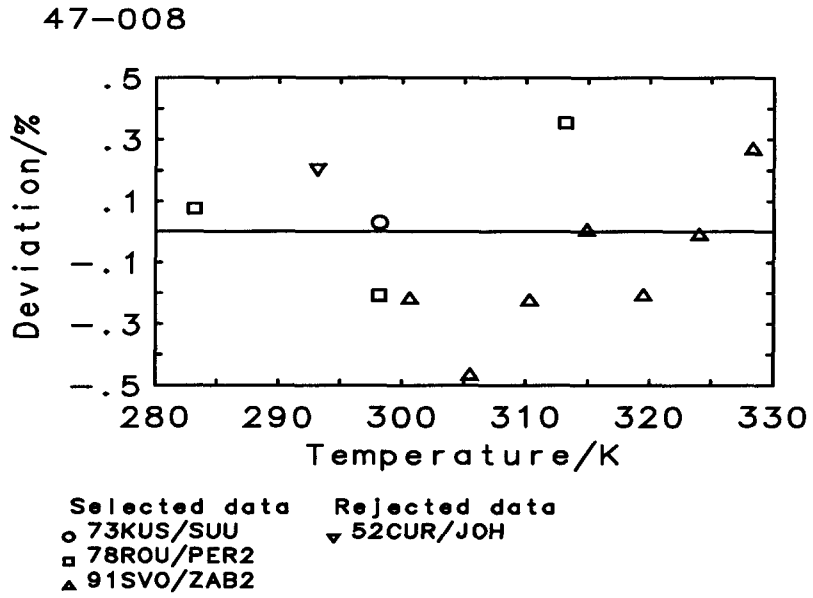
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KUS/SUU	298.1	1	0.10	0.273	6.91–3	0.03	6.91–3	1
78ROU/PER2	283.1–313.1	3	0.50#	0.481	6.22–2	0.24	1.89–2	1
91SVO/ZAB2	300.6–328.3	7	0.50	0.501	6.48–2	0.25	–3.23–2	–4
				Rejected data				
52CUR/JOH	(5.17–2, 0.21, 5.17–2, 1)			89COB/GAR	(4.25–1, 1.71, –4.25–1, –1)			

TABLE 47.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	11	0.530	6.75–2	0.26	–1.48–2	–2
Temp. range K		A_1	A_2				Level of uncertainty
283.1–328.3		1.17369+1	4.56463				III

TABLE 47.8.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.262	2.304	2.338	2.346	2.388	2.430	2.473
C_p (J K^{-1}mol^{-1})	203.9	207.6	210.7	211.4	215.2	219.0	222.8



Name: 2,2'–Oxybisethanol
Formula: $C_4H_{10}O_3$

CAS–RN: 111–46–6
Group No.: 47–009
Molar Mass: 106.12

TABLE 47.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
79STE/TAM		273.1–513.2	14S	nosp	99.9	chrom	C_{sat}	BDHT	69PER/COM

52CUR/JOH technical product, purity in question

TABLE 47.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79STE/TAM	273.1–513.2	14	1.00#	0.325	1.15–1	0.32	7.95–4	–2
				Rejected data				
52CUR/JOH	(2.46, 9.20,–2.46, –1)							

TABLE 47.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	14	0.384	1.36–1	0.38	7.95–4	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
273.1–513.2		4.21850+1	–1.87693+1	6.74201	–6.32894–1		IV

TABLE 47.9.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} ($J K^{-1} g^{-1}$)	2.209	2.219	2.240	2.274	2.302	2.309	2.345
C_{sat} ($J K^{-1} mol^{-1}$)	234.5	235.5	237.8	241.3	244.3	245.0	248.9
Temp. (K)	320	330	340	350	360	370	380
c_{sat} ($J K^{-1} g^{-1}$)	2.384	2.423	2.463	2.503	2.543	2.584	2.624
C_{sat} ($J K^{-1} mol^{-1}$)	253.0	257.1	261.3	265.6	269.9	274.2	278.4
Temp. (K)	390	400	410	420	430	440	450
c_{sat} ($J K^{-1} g^{-1}$)	2.663	2.701	2.738	2.773	2.806	2.837	2.866
C_{sat} ($J K^{-1} mol^{-1}$)	282.6	286.6	290.5	294.3	297.8	301.1	304.1
Temp. (K)	460	470	480	490	500	510	
c_{sat} ($J K^{-1} g^{-1}$)	2.891	2.914	2.933	2.948	2.960	2.967	
C_{sat} ($J K^{-1} mol^{-1}$)	306.8	309.2	311.3	312.9	314.1	314.8	

TABLE 47.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	15	14	0.694	2.45–1	0.69	3.02–3	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
273.1–513.2	760.00	2.85512+1	2.49786	7.55126	8.15873+1	IV

Name: 2–Furancarboxaldehyde
Formula: $C_5H_4O_2$

CAS–RN: 98–01–1
Group No.: 47–010
Molar Mass: 96.09

TABLE 47.10.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON		317.5–370.7	3S	nosp	not specified		C_{avg}	DSIO	*81VON
34MIL	N	256.0–267.9	2	nosp	not specified		C_{avg}	BSIO	20GIB/LAT
62OME2		288.6–422.0	6	nosp	not specified		C_p	not specified	
67RAS/GAN		293.1–373.1	5S	0.50	not specified		C_p	BSAO	67RAS/GAN

34MIL average values in temperature ranges 240–272 K and 262–274 K

TABLE 47.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67RAS/GAN	293.1–373.1	5	0.50	0.144	1.43–2	0.07	1.79–5	–1
				Rejected data				
*81VON	(2.25–1, 1.08, 2.10–1, 3)			62OME2	(2.89–1, 1.41, 2.78–1, 3)			

TABLE 47.10.3. Parameters of regression polynomial

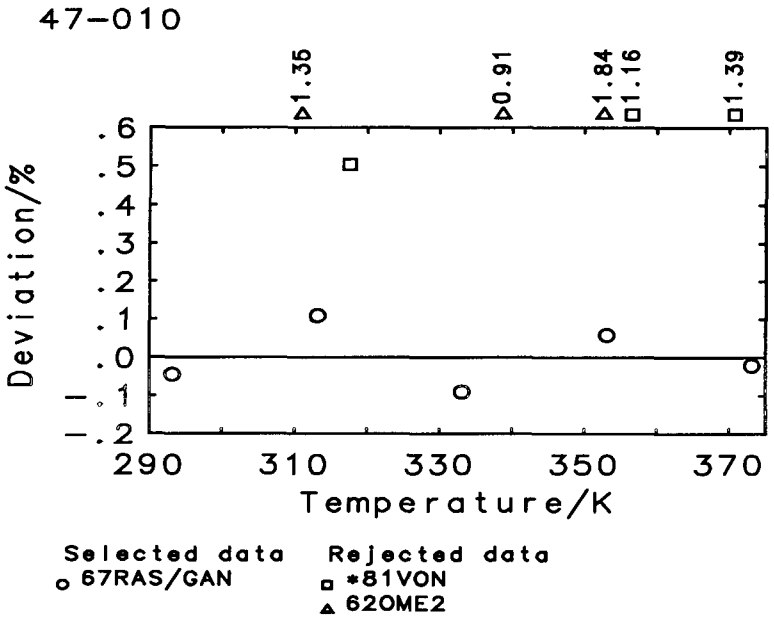
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	5	0.185	1.84–2	0.09	1.79–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
293.1–373.1	1.31948+1	2.04599	IV

TABLE 47.10.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.655	1.670	1.673	1.691	1.708	1.726	1.744
C_p (J K^{-1}mol^{-1})	159.0	160.4	160.7	162.4	164.1	165.8	167.5

Temp. (K)	350	360	370
c_p (J K^{-1}g^{-1})	1.761	1.779	1.797
C_p (J K^{-1}mol^{-1})	169.2	170.9	172.7



Name: 2–Furanmethanol
Formula: $C_5H_6O_2$

CAS–RN: 98–00–0
Group No.: 47–011
Molar Mass: 98.10

TABLE 47.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
34MIL	262.8	1	nosp	not specified		C_p	BSIO	20GIB/LAT
50HOU/MAS2	303.1–333.1	4S	0.40	99.8	estim	C_p	BSAO	50SAG/HOU
56PAR/KEN	260.0–300.0	5S	1.00	99.2	melpt	C_p	BSIO	25PAR

TABLE 47.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50HOU/MAS2	303.1–333.1	4	0.40	0.748	7.30–2	0.30	−2.94–2	0
56PAR/KEN	260.0–300.0	5	1.00	0.913	2.22–1	0.91	1.54–1	3
				Rejected data				
34MIL	(2.67, 13.32, −2.67, −1)							

TABLE 47.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	9	0.956	1.96–1	0.80	7.22–2	3
Temp. range K		A_1	A_2				Level of uncertainty
260.0–333.1		1.22271+1	4.00586				IV

TABLE 47.11.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.919	1.953	1.964	1.987	2.021	2.049	2.055
C_p (J K^{-1}mol^{-1})	188.3	191.6	192.6	194.9	198.3	201.0	201.6
Temp. (K)	310	320	330				
c_p (J K^{-1}g^{-1})	2.089	2.123	2.157				
C_p (J K^{-1}mol^{-1})	204.9	208.2	211.6				

Name: Tetrahydro–2*H*–pyran–2–one
Formula: $C_5H_8O_2$

CAS–RN: 542–28–9
Group No.: 47–012
Molar Mass: 100.12

TABLE 47.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83LEB/EVS	N	265.1–309.9	12	0.30	98.8	melpt	C_p	BSAO	76LEB/LIT

83LEB/EVS same data in 81EVS/LEB

TABLE 47.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.505	3.11–2	0.15	8.07–5	–2
Temp. range K		A_1	A_2				Level of uncertainty
265.1–309.9		1.27573+1	2.64720				III

TABLE 47.12.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.653	1.660	1.675	1.697	1.715	1.719	1.741
C_p (J K^{-1}mol^{-1})	165.5	166.2	167.7	169.9	171.7	172.1	174.3

Name: Tetrahydro–2–furanmethanol
Formula: $C_5H_{10}O_2$

CAS–RN: 97–99–4
Group No.: 47–013
Molar Mass: 102.13

TABLE 47.13.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76BON/CER	298.15	1.860	nosp	not specified		C_p	BSIO	76BON/CER

Name: 2–Methoxyethanol acetate
Formula: $C_5H_{10}O_3$

CAS–RN: 110–49–6
Group No.: 47–014
Molar Mass: 118.13

TABLE 47.14.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52CUR/JOH	303.15	2.075	nosp	not specified		C_p	not specified	

Name: 2–(1–Methylethoxy)ethanol
Formula: $C_5H_{12}O_2$

CAS–RN: 109–59–1
Group No.: 47–015
Molar Mass: 104.15

TABLE 47.15.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KUS/SUU	298.15	2.293	0.10	not specified		C_p	DDCT	71KON/SUU

Name: 2–Propoxyethanol
Formula: $C_5H_{12}O_2$

CAS–RN: 2807–30–9
Group No.: 47–016
Molar Mass: 104.15

TABLE 47.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KUS/SUU	298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
78ROU/PER2	298.1	1	nosp	99.	chrom	C_p	FSIT	71PIC/LED
91SVO/ZAB2	300.6–328.3	7	0.50	99.95	chrom	C_p	BSAO	91SVO/ZAB1

TABLE 47.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73KUS/SUU	298.1	1	0.10	0.044	1.28–3	0.00	–1.28–3	0
91SVO/ZAB2	300.6–328.3	7	0.50	0.257	3.85–2	0.13	4.65–3	1
				Rejected data				
78ROU/PER2	(3.24–1, 1.10, 3.24–1, 1)							

TABLE 47.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	8	0.279	4.16–2	0.14	3.91–3	1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–328.3		1.39598+1	5.06427				III

TABLE 47.16.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.287	2.320	2.327	2.368	2.408	2.449
C_p (J K^{-1}mol^{-1})	238.2	241.6	242.4	246.6	250.8	255.0

Name: 2–(2–Methoxyethoxy)ethanol
Formula: $C_5H_{12}O_3$

CAS–RN: 111–77–3
Group No.: 47–017
Molar Mass: 120.15

TABLE 47.17.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
89COB/GAR		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question

TABLE 47.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
52CUR/JOH	293.1	1	3.00#	0.000	0.00	0.00	0.00	0
89COB/GAR	298.1	1	0.50#	0.000	0.00	0.00	0.00	0

TABLE 47.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–298.1		4.76392	8.97591				V

TABLE 47.17.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	2.13	2.18	2.19
C_p (J K^{-1}mol^{-1})	256	262	264

Name: 3,6–Dimethyl–1,4–dioxane–2,5–dione
Formula: $C_6H_8O_4$

CAS–RN: 95–96–5
Group No.: 47–018
Molar Mass: 144.13

TABLE 47.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80KUL/LEB	N	397.5–430.0	3S	nosp	not specified		C_p	not specified	

80KUL/LEB error of 0.1–0.3 % reported in 84VAS/PET

TABLE 47.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.015	5.43–3	0.02	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
397.5–430.0	3.50421+1	1.74660–1	IV

TABLE 47.18.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430
c_p ($J\,K^{-1}g^{-1}$)	2.062	2.063	2.064	2.065
C_p ($J\,K^{-1}mol^{-1}$)	297.2	297.3	297.5	297.6

Name: 2–Oxepanone
Formula: $C_6H_{10}O_2$

CAS–RN: 502–44–3
Group No.: 47–019
Molar Mass: 114.14

TABLE 47.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83LEB/EVS	269.9–327.8	16	0.30	99.35	melpt	C_p	BSAO	76LEB/LIT

TABLE 47.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.456	3.31–2	0.14	8.49–5	0

Temp. range K	A_1	A_2	Level of uncertainty
269.9–327.8	1.19875+1	3.91517	II

TABLE 47.19.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	1.643	1.652	1.672	1.700	1.723	1.729	1.757
C_p ($J K^{-1}mol^{-1}$)	187.6	188.6	190.8	194.1	196.7	197.3	200.6
Temp. (K)	320	330					
c_p ($J K^{-1}g^{-1}$)	1.786	1.814					
C_p ($J K^{-1}mol^{-1}$)	203.8	207.1					

Name: Ethyl ester 3–oxobutanoic acid
Formula: $C_6H_{10}O_3$

CAS–RN: 141–97–9
Group No.: 47–020
Molar Mass: 130.14

TABLE 47.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON		315.7–376.2	5S	nosp	not specified		C_{avg}	DSIO	*81VON
34KOL/UDO2	N	297.5	1	nosp	not specified		C_p	BSIT	34KOL/UDO2

34KOL/UDO2 same datum in 33KOL/UDO

TABLE 47.20.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	315.7–376.2	5	3.00#	0.002	1.61–3	0.01	0.00	0

TABLE 47.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	5	0.002	2.08–3	0.01	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
315.7–376.2		1.63275+1	4.26647				V

TABLE 47.20.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1}g^{-1}$)	1.92	1.94	1.97	2.00	2.02	2.05	2.08
C_p ($J K^{-1}mol^{-1}$)	249	253	256	260	263	267	271

Name: Tetrahydro–2*H*–pyran–2–methanol
Formula: $C_6H_{12}O_2$

CAS–RN: 100–72–1
Group No.: 47–021
Molar Mass: 116.16

TABLE 47.21.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76BON/CER	298.15	1.911	nosp	not specified		C_p	BSIO	76BON/CER

Name: 2–Ethoxyethanol acetate
Formula: $C_6H_{12}O_3$

CAS–RN: 111–15–9
Group No.: 47–022
Molar Mass: 132.16

TABLE 47.22.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52CUR/JOH	293.15	2.067	nosp	not specified		C_p	not specified	

Name: 2–Butoxyethanol
Formula: $C_6H_{14}O_2$

CAS–RN: 111–76–2
Group No.: 47–023
Molar Mass: 118.18

TABLE 47.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
59ONK		298.1–373.1	16S	nosp	not specified		C_p	BSAO	59ONK
73KUS/SUU		298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
78ROU/PER2		277.1–328.1	5	nosp	99.	chrom	C_p	FSIT	71PIC/LED
89COB/GAR		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question

TABLE 47.23.2. Correlated heat capacities

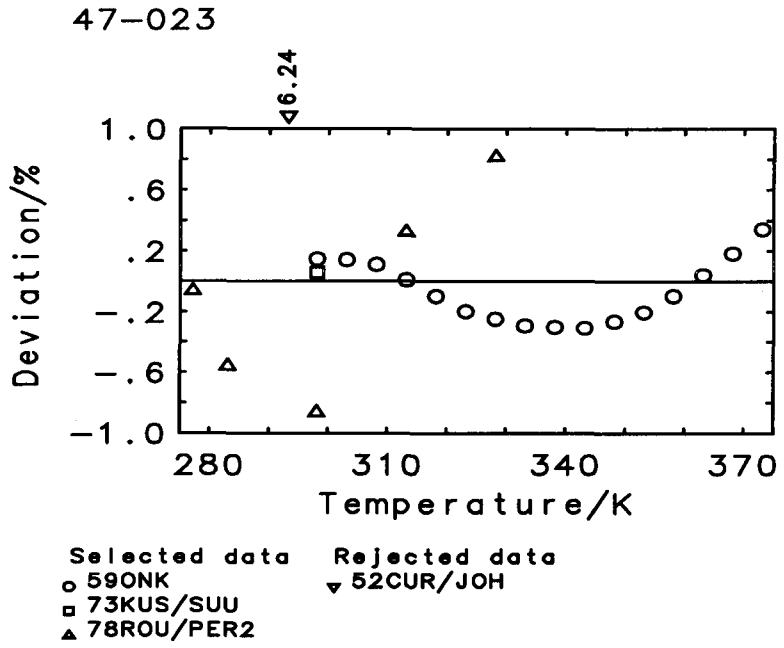
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59ONK	298.1–373.1	16	0.50#	0.422	7.45–2	0.21	–2.32–2	–3
73KUS/SUU	298.1	1	0.10	0.579	1.90–2	0.06	1.90–2	1
78ROU/PER2	277.1–328.1	5	0.50#	1.211	2.02–1	0.61	–1.74–2	–1
				Rejected data				
52CUR/JOH	(2.16, 6.24, 2.16, 1)		89COB/GAR	(4.81–1, 1.49,–4.81–1, –1)				

TABLE 47.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	22	0.744	1.24–1	0.37	–2.00–2	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
277.1–373.1		1.77995	1.44841+1	–1.36536			III

TABLE 47.23.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.225	2.273	2.310	2.318	2.361	2.403	2.442
C_p (J K^{-1}mol^{-1})	263.0	268.6	272.9	273.9	279.0	283.9	288.6
Temp. (K)	340	350	360	370			
c_p (J K^{-1}g^{-1})	2.480	2.515	2.549	2.581			
C_p (J K^{-1}mol^{-1})	293.0	297.2	301.2	305.0			



Name: 2-(2-Ethoxyethoxy)ethanol
Formula: $C_6H_{14}O_3$

CAS-RN: 111-90-0
Group No.: 47-024
Molar Mass: 134.18

TABLE 47.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
89COB/GAR		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question

TABLE 47.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89COB/GAR	298.1	1	1.00#	0.000	0.00	0.00	0.00	0

TABLE 47.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	3.57495+1	V

TABLE 47.24.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.22
C_p (J K^{-1}mol^{-1})	297

Name: 2,2'–[1,2–Ethanediylbis(oxy)]bisethanol
Formula: $C_6H_{14}O_4$

CAS–RN: 112–27–6
Group No.: 47–025
Molar Mass: 150.17

TABLE 47.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
79STE/TAM		273.1–533.2	15S	nosp	99.9	chrom	C_{sat}	BDHT	69PER/COM

52CUR/JOH technical product, purity in question

TABLE 47.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
79STE/TAM	273.1–533.2	15	1.00#	0.454	2.25–1	0.45	2.03–3	–3
				Rejected data				
52CUR/JOH	(6.70–1, 1.69, 6.70–1, 1)							

TABLE 47.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	15	0.530	2.63–1	0.53	2.03–3	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
273.1–533.2		5.21263+1	–2.36376+1	9.16050	–8.95123–1		IV

TABLE 47.25.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.074	2.085	2.110	2.147	2.179	2.186	2.227
C_{sat} (J K^{-1}mol^{-1})	311.5	313.2	316.9	322.5	327.2	328.3	334.4
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.268	2.309	2.351	2.394	2.435	2.477	2.517
C_{sat} (J K^{-1}mol^{-1})	340.5	346.8	353.1	359.5	365.7	371.9	378.0
Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	2.556	2.594	2.630	2.664	2.696	2.725	2.751
C_{sat} (J K^{-1}mol^{-1})	383.9	389.6	395.0	400.1	404.9	409.2	413.1
Temp. (K)	460	470	480	490	500	510	520
c_{sat} (J K^{-1}g^{-1})	2.774	2.793	2.809	2.820	2.827	2.829	2.826
C_{sat} (J K^{-1}mol^{-1})	416.6	419.5	421.8	423.5	424.5	424.9	424.4
Temp. (K)	530						
c_{sat} (J K^{-1}g^{-1})	2.818						
C_{sat} (J K^{-1}mol^{-1})	423.2						

TABLE 47.25.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	15	0.883	4.12–1	0.88	6.81–3	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
273.1–533.2	728.00	6.42875+1	6.81337	–3.33237–1	1.51646+2		IV

Name: 2-Hydroxybenzaldehyde
Formula: $C_7H_6O_2$

CAS-RN: 90-02-8
Group No.: 47-026
Molar Mass: 122.12

TABLE 47.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
04LOU	N	382.4	1	nosp	not specified		C_{avg}	DSIO	*98LOU
07WAL		291.1	1	nosp	not specified		C_p	DSIO	07WAL

04LOU average value in temperature range 297–468 K; average of 3 measurements

TABLE 47.26.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
04LOU	382.4	1	5.00#	0.000	0.00	0.00	0.00	0
07WAL	291.1	1	5.00#	0.000	0.00	0.00	0.00	0

TABLE 47.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
291.1–382.4		9.45577	4.81534				VI

TABLE 47.26.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.59	1.62	1.63	1.66	1.69	1.73	1.76
C_p ($J K^{-1} mol^{-1}$)	195	198	199	203	207	211	215
Temp. (K)	350	360	370	380			
c_p ($J K^{-1} g^{-1}$)	1.79	1.82	1.86	1.89			
C_p ($J K^{-1} mol^{-1}$)	219	223	227	231			

Name: 2–Hydroxybenzoic acid
Formula: $C_7H_6O_3$

CAS–RN: 69–72–7
Group No.: 47–027
Molar Mass: 138.12

TABLE 47.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86RAB/SHE	439.6–459.5	14	1.50	99.84	melpt	C_p	BSAO	68LEA

TABLE 47.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.279	1.56–1	0.42	1.37–3	–2
Temp. range K		A_1	A_2				Level of uncertainty
439.6–459.5		–1.25651+2	3.62422+1				V

TABLE 47.27.4. Recommended values of heat capacities

Temp. (K)	440	450	460
c_p ($J K^{-1} g^{-1}$)	2.04	2.25	2.47
C_p ($J K^{-1} mol^{-1}$)	281	311	341

Name: 2,6–Dimethyl–4*H*–pyran–4–one
Formula: $C_7H_8O_2$

CAS–RN: 1004–36–0
Group No.: 47–028
Molar Mass: 124.14

TABLE 47.28.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
11POM	N	439.05	2.301	nosp	not specified		C_{avg}	DSIO	11POM

11POM average value in temperature range 425–453 K

Name: Methyl 2–hydroxybenzoate
Formula: $C_8H_8O_3$

CAS–RN: 119–36–8
Group No.: 47–029
Molar Mass: 152.15

TABLE 47.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
33KOL/UDO	295.1	1	nosp	not specified		C_p	BSIT	34KOL/UDO2
34KOL/UDO2	295.1	1	nosp	not specified		C_p	BSIT	34KOL/UDO2

TABLE 47.29.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
33KOL/UDO	295.1	1	3.00#	0.000	0.00	0.00	0.00	0
				Rejected data				
34KOL/UDO2	(2.37, 7.90,–2.37, –1)							

TABLE 47.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
295.1–295.1		3.22864+1					VI

TABLE 47.29.4. Recommended values of heat capacities

Temp. (K)	295.15
c_p ($J K^{-1}g^{-1}$)	1.76
C_p ($J K^{-1}mol^{-1}$)	268

Name: 2–Phenoxyethanol
Formula: $C_8H_{10}O_2$

CAS–RN: 122–99–6
Group No.: 47–030
Molar Mass: 138.17

TABLE 47.30.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75NIC/WAD	298.15	2.132	nosp	99.5	chrom	C_p	BSIO	70LKB/COM

Name: Diethyl ester 2,3–dihydroxy–[*R*–(*R**,*R**)]–butanedioic acid
Formula: $C_8H_{14}O_6$

CAS–RN: 87–91–2
Group No.: 47–031
Molar Mass: 206.20

TABLE 47.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
30WAS2	335.5–335.8	2	2.00	not specified		C_{avg}	DSIO	30WAS1

TABLE 47.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.760	7.34–1	1.52	1.12–2	0

Temp. range K	A_1	Level of uncertainty
335.5–335.8	4.82377+1	V

TABLE 47.31.4. Recommended values of heat capacities

Temp. (K)	340
c ($J K^{-1}g^{-1}$)	1.95
C ($J K^{-1}mol^{-1}$)	401

Name: 2–(2–Ethoxyethoxy)ethanol acetate
Formula: $C_8H_{16}O_4$

CAS–RN: 112–15–2
Group No.: 47–032
Molar Mass: 176.21

TABLE 47.32.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	293.15	2.251	nosp	not specified		C_p	not specified	

52CUR/JOH technical product, purity in question

Name: 2–(2–Butoxyethoxy)ethanol
Formula: $C_8H_{18}O_3$

CAS–RN: 112–34–5
Group No.: 47–033
Molar Mass: 162.23

TABLE 47.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52CUR/JOH	N	293.1	1	nosp	not specified		C_p	not specified	
87COB/CAS		298.1	1	nosp	98.	anal	C_p	FSIT	71PIC/LED

52CUR/JOH technical product, purity in question

TABLE 47.33.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
87COB/CAS	298.1	1	0.50#	0.000	0.00	0.00	0.00	0

TABLE 47.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	4.26832+1	IV

TABLE 47.33.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.188
C_p (J K^{-1}mol^{-1})	354.9

Name: 2,2'–[Oxybis(2,1–ethanediyloxy)]bisethanol
Formula: $C_8H_{18}O_5$

CAS–RN: 112–60–7
Group No.: 47–034
Molar Mass: 194.23

TABLE 47.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79STE/TAM	273.1–533.2	14S	nosp	99.9	chrom	C_{sat}	BDHT	69PER/COM

TABLE 47.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	14	14	0.083	4.37–2	0.08	5.42–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.1–533.2		1.44251+1	1.56386+1	−1.17879			IV

TABLE 47.34.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	2.057	2.070	2.096	2.135	2.165	2.172	2.208
C_{sat} (J K^{-1}mol^{-1})	399.6	402.0	407.2	414.6	420.5	421.8	428.8
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.243	2.277	2.310	2.342	2.374	2.404	2.433
C_{sat} (J K^{-1}mol^{-1})	435.7	442.3	448.7	455.0	461.0	466.9	472.5
Temp. (K)	390	400	410	420	430	440	450
c_{sat} (J K^{-1}g^{-1})	2.461	2.488	2.514	2.539	2.563	2.586	2.608
C_{sat} (J K^{-1}mol^{-1})	478.0	483.2	488.3	493.2	497.8	502.3	506.6
Temp. (K)	460	470	480	490	500	510	520
c_{sat} (J K^{-1}g^{-1})	2.629	2.649	2.668	2.686	2.703	2.719	2.734
C_{sat} (J K^{-1}mol^{-1})	510.7	514.6	518.3	521.7	525.0	528.2	531.1
Temp. (K)	530						
c_{sat} (J K^{-1}g^{-1})	2.748						
C_{sat} (J K^{-1}mol^{-1})	533.8						

TABLE 47.34.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	14	14	0.160	9.13–2	0.16	8.23–5	−1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
273.1–533.2	730.00	3.95425+1	3.31314	1.75309+1	1.17986+2	IV

Name: 1,3–Dihydro–1,3–dioxo–5–isobenzofurancarboxylic acid
Formula: $C_9H_4O_5$

CAS–RN: 552–30–7
Group No.: 47–035
Molar Mass: 192.13

TABLE 47.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78MAR/CIO2	N	390.0–540.0	16S	nosp	not specified		C_p	DSIO	71MAR/CIO

78MAR/CIO2 values calculated from temperature dependence of enthalpy by the authors

Name: (Phenoxymethyl)oxirane
Formula: $C_9H_{10}O_2$

CAS–RN: 122–60–1
Group No.: 47–036
Molar Mass: 150.18

TABLE 47.36.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87LES/LIC	240.0–390.0	eqn	2.00	99.	estim	C_p	BDHT	69PER/COM

TABLE 47.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.000	1.40–5	0.00	–7.15–7	0

Temp. range K	A_1	A_2	Level of uncertainty
240.0–390.0	2.64429+1	2.37427	V

TABLE 47.36.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	1.78	1.79	1.81	1.82	1.82	1.83	1.85
C_p ($J K^{-1}mol^{-1}$)	267	269	271	273	274	275	277
Temp. (K)	298.15	300	310	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	1.86	1.86	1.87	1.88	1.90	1.91	1.92
C_p ($J K^{-1}mol^{-1}$)	279	279	281	283	285	287	289
Temp. (K)	360	370	380	390			
c_p ($J K^{-1}g^{-1}$)	1.94	1.95	1.96	1.98			
C_p ($J K^{-1}mol^{-1}$)	291	293	295	297			

Name: 2–Methoxy–4–(2–propenyl)phenol
Formula: $C_{10}H_{12}O_2$

CAS–RN: 97–53–0
Group No.: 47–037
Molar Mass: 164.20

TABLE 47.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83KAR/ABD1	273.0–293.0	2	nosp	not specified		C_p	BSAO	82KAR/IGA

TABLE 47.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
273.0–293.0	–9.35613	1.72805+1	V

TABLE 47.37.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15
c_p ($J\,K^{-1}g^{-1}$)	1.89	1.92	1.98	2.06	2.14
C_p ($J\,K^{-1}mol^{-1}$)	310	315	325	339	351

Name: 2-(2-Butoxyethoxy)ethanol acetate
Formula: $C_{10}H_{20}O_4$

CAS-RN: 124-17-4
Group No.: 47-038
Molar Mass: 204.27

TABLE 47.38.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52CUR/JOH	N	301.15	2.008	nosp	not specified		C_p	not specified	

52CUR/JOH technical product, purity in question

Name: 3,6,9,12-Tetraoxatetradecane-1,14-diol
Formula: $C_{10}H_{22}O_6$

CAS-RN: 4792-15-8
Group No.: 47-039
Molar Mass: 238.28

TABLE 47.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79STE/TAM	273.1-513.2	13S	nosp	99.1	chrom	C_{sat}	BDHT	69PER/COM

TABLE 47.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	13	13	0.042	3.09-2	0.04	-3.58-5	3

Temp. range K	A_1	A_2	Level of uncertainty
273.1-513.2	4.42361+1	5.97792	IV

TABLE 47.39.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} ($J\,K^{-1}g^{-1}$)	2.107	2.113	2.128	2.148	2.165	2.169	2.190
C_{sat} ($J\,K^{-1}mol^{-1}$)	502.0	503.6	507.0	511.9	516.0	516.9	521.9
Temp. (K)	320	330	340	350	360	370	380
c_{sat} ($J\,K^{-1}g^{-1}$)	2.211	2.232	2.253	2.274	2.294	2.315	2.336
C_{sat} ($J\,K^{-1}mol^{-1}$)	526.9	531.8	536.8	541.8	546.7	551.7	556.7
Temp. (K)	390	400	410	420	430	440	450
c_{sat} ($J\,K^{-1}g^{-1}$)	2.357	2.378	2.399	2.420	2.441	2.461	2.482
C_{sat} ($J\,K^{-1}mol^{-1}$)	561.6	566.6	571.6	576.6	581.5	586.5	591.5
Temp. (K)	460	470	480	490	500	510	
c_{sat} ($J\,K^{-1}g^{-1}$)	2.503	2.524	2.545	2.566	2.587	2.607	
C_{sat} ($J\,K^{-1}mol^{-1}$)	596.4	601.4	606.4	611.3	616.3	621.3	

Name: Oxacyclododecan–2–one
Formula: $C_{11}H_{20}O_2$

CAS–RN: 1725–03–7
Group No.: 47–040
Molar Mass: 184.28

TABLE 47.40.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81LEB/EVS1	N	278.7–336.6	14	0.30	not specified		C_p	BSAO	76LEB/LIT

81LEB/EVS1 same data in 81LEB/EVS2

TABLE 47.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	0.296	3.82–2	0.09	5.26–5	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
278.7–336.6	2.73252+1	1.87318	9.30682–1	III

TABLE 47.40.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.799	1.831	1.858	1.864	1.898	1.933	1.969
C_p (J K^{-1}mol^{-1})	331.5	337.4	342.4	343.6	349.8	356.3	362.9

Temp. (K)	340
c_p (J K^{-1}g^{-1})	2.006
C_p (J K^{-1}mol^{-1})	369.6

Name: Phenyl ester 2–hydroxybenzoic acid
Formula: $C_{13}H_{10}O_3$

CAS–RN: 118–55–8
Group No.: 47–041
Molar Mass: 214.22

TABLE 47.41.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
13CAM	N	317.25	1.635	nosp	not specified		C_p	not specified	

13CAM error 0.5 % (information in 29WAS)

Name: Oxacyclotetradecan–2–one
Formula: $C_{13}H_{24}O_2$

CAS–RN: 1725–04–8
Group No.: 47–042
Molar Mass: 212.33

TABLE 47.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81LEB/EVS1	301.8–329.2	9	0.30	99.85	melpt	C_p	BSAO	76LEB/LIT

TABLE 47.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.300	4.46–2	0.09	5.55–5	1
Temp. range K		A_1	A_2				Level of uncertainty
301.8–329.2		1.42778+1	1.12705+1				II

TABLE 47.42.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p (J $K^{-1}g^{-1}$)	1.883	1.927	1.971	2.015
C_p (J $K^{-1}mol^{-1}$)	399.8	409.2	418.6	428.0

Name: 1–[4–(1,1–Diethoxyethyl)phenyl]ethanone
Formula: $C_{14}H_{20}O_3$

CAS–RN: 64533–95–5
Group No.: 47–043
Molar Mass: 236.31

TABLE 47.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78KAR/RAB	331.1–337.3	7	0.20	99.0	melpt	C_p	BSAO	76LEB/LIT

TABLE 47.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.477	6.86–2	0.10	9.26–5	0
Temp. range K		A_1	A_2				Level of uncertainty
331.1–337.3		3.98293+1	9.66719				III

TABLE 47.43.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p (J $K^{-1}g^{-1}$)	2.524	2.558
C_p (J $K^{-1}mol^{-1}$)	596.4	604.4

Name: Oxacyclohexadecan–2–one
Formula: $C_{15}H_{28}O_2$

CAS–RN: 106–02–5
Group No.: 47–044
Molar Mass: 240.39

TABLE 47.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81LEB/EVS1	N	309.3–326.3	7	0.30	99.8	melpt	C_p	BSAO	76LEB/LIT

81LEB/EVS1 same data in 79LEB/EVS

TABLE 47.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.440	7.50–2	0.13	1.41–4	0
Temp. range K		A_1	A_2				Level of uncertainty
309.3–326.3		2.54321+1	1.00272+1				II

TABLE 47.44.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p (J K^{-1}g^{-1})	1.955	1.989	2.024
C_p (J K^{-1}mol^{-1})	469.9	478.2	486.6

Name: 2,2'–[(1–Methylethylidene)bis(4,1–phenyleneoxymethylene)]bisoxirane
Formula: $C_{21}H_{24}O_4$

CAS–RN: 1675–54–3
Group No.: 47–045
Molar Mass: 340.42

TABLE 47.45.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	%	Purity method	Type capacity	Calorimeter Type	Reference
87LES/LIC	N	280.0–360.0	eqn	2.00	99.	estim	C_p	BDHT	69PER/COM

87LES/LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 47.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.000	3.50–5	0.00	2.54–6	0
Temp. range K		A_1	A_2				Level of uncertainty
280.0–360.0		4.85772+1	8.79720				V

TABLE 47.45.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.79	1.81	1.83	1.83	1.85	1.87	1.90
C_p (J K^{-1}mol^{-1})	609	616	622	623	631	638	645
Temp. (K)	340	350	360				
c_p (J K^{-1}g^{-1})	1.92	1.94	1.96				
C_p (J K^{-1}mol^{-1})	653	660	667				

Name: 2,3–Dihydroxypropyl ester octadecanoic acid
Formula: $C_{21}H_{42}O_4$

CAS–RN: 123–94–4
Group No.: 47–046
Molar Mass: 358.56

TABLE 47.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55WAR/VIC	360.5–387.5	6	1.00	99.	melpt	C_p	BSAO	44BAI/TOD

TABLE 47.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.778	9.42–1	0.78	9.42–3	0
Temp. range K		A_1	A_2				Level of uncertainty
360.5–387.5		–2.67652+1	4.06099+1				IV

TABLE 47.46.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390
c_p (J K^{-1}g^{-1})	2.769	2.864	2.958	3.052
C_p (J K^{-1}mol^{-1})	993.0	1027	1061	1094

Name: *trans*–Bis(4–methoxyphenyl)ester 1,4–cyclohexanedicarboxylic acid
Formula: $C_{22}H_{24}O_6$

CAS–RN: 26379–55–5
Group No.: 47–047
Molar Mass: 384.43

TABLE 47.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74AND/BAC	519.6–547.3	12	0.10	99.82	melpt	C_{sat}	BSAO	53WES/HAT

TABLE 47.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	8.010	8.35–1	0.80	1.11–2	–2
Temp. range K		A_1	A_2				Level of uncertainty
519.6–547.3		5.47618+1	9.28946				IV

TABLE 47.47.4. Recommended values of heat capacities

Temp. (K)	520	530	540	550
c_{sat} (J K^{-1}g^{-1})	2.229	2.249	2.269	2.289
C_{sat} (J K^{-1}mol^{-1})	857.0	864.7	872.4	880.1

Name: 3-(Acetyloxy)-2-hydroxypropyl ester octadecanoic acid
Formula: $C_{23}H_{44}O_5$

CAS-RN: 820-17-7
Group No.: 47-048
Molar Mass: 400.60

TABLE 47.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55WAR/VIC	333.1–345.3	4	1.00	98.	melpt	C_p	BSAO	44BAI/TOD

TABLE 47.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	4	0.679	9.15-1	0.68	5.81-3	-2
Temp. range K		A_1	A_2				Level of uncertainty
333.1–345.3		-3.14211+2	1.32999+2				IV

TABLE 47.48.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_p (J K^{-1}g^{-1})	2.588	2.864	3.140
C_p (J K^{-1}mol^{-1})	1037	1147	1258

Name: 4-(Heptyloxy)phenyl ester 4-butylbenzoic acid
Formula: $C_{24}H_{32}O_3$

CAS-RN: 38454-35-2
Group No.: 47-049
Molar Mass: 368.52

TABLE 47.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85SHA/ZHU	328.3–354.5	6	0.50	not specified		C_p	BSAO	87KHO/BUG

TABLE 47.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.392	1.76-1	0.20	4.64-4	0
Temp. range K		A_1	A_2				Level of uncertainty
328.3–354.5		6.81699+1	6.38683				III

TABLE 47.49.4. Recommended values of heat capacities

Temp. (K)	330	340	350
c_p (J K^{-1}g^{-1})	2.014	2.028	2.042
C_p (J K^{-1}mol^{-1})	742.0	747.4	752.7

Name: 4–(Hexyloxy)phenyl ester 4–(decyloxy)benzoic acid
Formula: $C_{29}H_{42}O_4$

CAS–RN: 68162–09–4
Group No.: 47–050
Molar Mass: 454.65

TABLE 47.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83ANI/VOR	N	364.0–394.5	5	nosp	99.7	melpt	C_p	BSAO	83ANI/VOR

83ANI/VOR data from a graph only

TABLE 47.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	1.521	1.75	1.52	2.22–2	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
364.0–394.5	4.38097+3	–2.21612+3	2.87419+2	V

TABLE 47.50.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_p (J K^{-1}g^{-1})	2.12	2.01	2.01
C_p (J K^{-1}mol^{-1})	965	915	913

Name: 3,4–Dihydro–2,5,7,8–tetramethyl–2–(4,8,12–trimethyltridecyl)acetate 2*H*–1–benzopyran–6–ol
Formula: $C_{31}H_{52}O_3$

CAS–RN: 7695–91–2
Group No.: 47–051
Molar Mass: 472.75

TABLE 47.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86BER/GUR	N	273.0–333.6	4	2.00	99.	estim	C_p	BDHT	86CDA/COM

86BER/GUR same data in 88BAG/GUR

TABLE 47.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.395	8.93–1	0.79	6.76–3	0

Temp. range K	A_1	A_2	Level of uncertainty
273.0–333.6	4.69175+1	2.09895+1	V

TABLE 47.51.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	1.82	1.83	1.86	1.90	1.93	1.93	1.97
C_p ($J K^{-1} mol^{-1}$)	861	867	879	896	910	914	931
Temp. (K)	320	330					
c_p ($J K^{-1} g^{-1}$)	2.01	2.04					
C_p ($J K^{-1} mol^{-1}$)	949	966					

51. Sulfides

The sulfide family contains 28 compounds, all of which but one were measured over a range of temperatures.

Most measurements of heat capacities for this family were carried out at BMB. Altogether 15 compounds were investigated (50SCO/FIN1, 51SCO/FIN, 52SCO/FIN1, 52SCO/FIN2, 55MCC/FIN, 57SCO/FIN, 58HUB/DOU, 61MCC/FIN, 62SCO/GOO, 67MES/TOD, 74MES/FIN) with a reported error of 0.2% which appears to be a realistic estimate.

Another large group of 14 compounds was measured in an unidentified fSU laboratory in Kazakhstan; the results were published as smoothed data and/or parameters of a quadratic temperature dependence (80TUT/GAB, 82TUT/GAB). These results differ enormously from those measured at BMB; the shape of the $C_p = f(T)$ curve is quite different. For this reason, the above data have been used only when no other data were available and a significant error in the recommended values has to be expected.

In addition to the above mentioned data from the two laboratories only two more measurements are available; reliable data for dimethyl sulfide from CITP (42OSB/DOE) with a somewhat unrealistically low uncertainty of 0.1% reported by the authors and one data set for phenyl methyl sulfide from JHUB (31SMI/AND2) where a sample of low purity was used for the measurements.

Name: Thiobismethane
Formula: C_2H_6S

CAS-RN: 75-18-3
Group No.: 51-001
Molar Mass: 62.14

TABLE 51.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
42OSB/DOE	181.2–286.7	14	0.10	99.993	melpt	C_p	BSAO	41YOS/GAR

TABLE 51.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	14	14	0.252	3.41–3	0.03	1.77–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
181.2–286.7		1.74001+1	–4.21426	1.29294	–7.97947–2		II

TABLE 51.1.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.812	1.808	1.807	1.808	1.811	1.817	1.824
C_p (J K^{-1}mol^{-1})	112.6	112.4	112.3	112.4	112.6	112.9	113.3
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.833	1.844	1.857	1.861	1.871	1.888	1.902
C_p (J K^{-1}mol^{-1})	113.9	114.6	115.4	115.7	116.3	117.3	118.2

TABLE 51.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	14	1.443	1.97–2	0.14	4.35–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
181.2–286.7	503.00	2.95281+1	1.03463+1	2.93747	2.10681+1		II

Name: 2,3–Dithiabutane
Formula: $C_2H_6S_2$

CAS–RN: 624–92–0
Group No.: 51–002
Molar Mass: 94.20

TABLE 51.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
50SCO/FIN1	192.0–352.3	25	0.20	99.97	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.2.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.175	6.09–3	0.03	3.20–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
192.0–270.0		2.50263+1	–8.32463	2.73276	–2.61467–1		II
270.0–352.3		2.08187+1	–3.64951	1.00122	–4.76980–2		II

TABLE 51.2.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.525	1.520	1.516	1.514	1.514	1.516	1.519
C_{sat} (J K^{-1}mol^{-1})	143.7	143.1	142.8	142.6	142.6	142.8	143.1
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.523	1.529	1.531	1.536	1.544	1.551	1.553
C_{sat} (J K^{-1}mol^{-1})	143.5	144.1	144.2	144.7	145.4	146.1	146.3
Temp. (K)	310	320	330	340	350		
c_{sat} (J K^{-1}g^{-1})	1.563	1.574	1.586	1.598	1.612		
C_{sat} (J K^{-1}mol^{-1})	147.2	148.2	149.4	150.6	151.9		

TABLE 51.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	19	0.605	2.12–2	0.12	4.17–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
219.3–352.3	606.00	1.48968+1	7.00541	9.96705	7.91943		II

Name: (Methylthio)ethane
Formula: C_3H_8S

CAS–RN: 624–89–5
Group No.: 51–003
Molar Mass: 76.16

TABLE 51.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
51SCO/FIN	171.9–297.6	18	0.20	99.9984	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.214	7.04–3	0.04	3.50–6	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
171.9–297.6		2.15639+1	–6.32172	2.16466	–1.72267–1		II

TABLE 51.3.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.771	1.768	1.767	1.769	1.773	1.779	1.788
C_{sat} (J K^{-1}mol^{-1})	134.9	134.6	134.6	134.7	135.0	135.5	136.2
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.799	1.812	1.827	1.843	1.849	1.862	1.881
C_{sat} (J K^{-1}mol^{-1})	137.0	138.0	139.1	140.4	140.8	141.8	143.3
Temp. (K)	298.15	300					
c_{sat} (J K^{-1}g^{-1})	1.899	1.903					
C_{sat} (J K^{-1}mol^{-1})	144.6	144.9					

TABLE 51.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	15	0.737	2.43–2	0.15	5.48–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
186.5–297.6	533.00	2.04293+1	9.42329	6.58582	1.10725+1		II

Name: 1–(Methylthio)propane
Formula: $C_4H_{10}S$

CAS–RN: 3877–15–4
Group No.: 51–004
Molar Mass: 90.19

TABLE 51.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
57SCO/FIN	167.4–325.8	20	0.20	99.98	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.4.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.143	5.54–3	0.03	2.48–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
167.4–255.0		2.38100+1	–5.90705	2.05285	–1.42628–1		II
255.0–325.8		2.75014+1	–1.02498+1	3.75589	–3.65248–1		II

TABLE 51.4.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J $K^{-1}g^{-1}$)	1.752	1.751	1.753	1.758	1.764	1.773	1.784
C_{sat} (J $K^{-1}mol^{-1}$)	158.0	157.9	158.1	158.5	159.1	159.9	160.9
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J $K^{-1}g^{-1}$)	1.796	1.811	1.827	1.845	1.851	1.865	1.886
C_{sat} (J $K^{-1}mol^{-1}$)	162.0	163.3	164.8	166.4	167.0	168.2	170.1
Temp. (K)	298.15	300	310	320	330		
c_{sat} (J $K^{-1}g^{-1}$)	1.904	1.908	1.930	1.954	1.978		
C_{sat} (J $K^{-1}mol^{-1}$)	171.7	172.1	174.1	176.2	178.4		

TABLE 51.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	20	20	1.494	5.94-2	0.30	2.85-4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
167.4–325.8	563.00	1.67004+1	9.46959	9.15500	7.36317		III

Name: 2-(Methylthio)propane
Formula: $C_4H_{10}S$

CAS-RN: 1551-21-9
Group No.: 51-005
Molar Mass: 90.19

TABLE 51.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
55MCC/FIN	177.2–343.8	22	0.20	99.982	melpt	C_{sat}	BSAO	43RUE/HUF
80TUT/GAB	273.1–343.1	8S	0.40	not specified		C_p	BSAO	62KOL/SER

TABLE 51.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
55MCC/FIN	177.2–343.8	22	0.20	0.113	4.66-3	0.02	3.12-6	1
				Rejected data				
80TUT/GAB	(7.92-1, 3.50, 6.23-1, 6)							

TABLE 51.5.3. Parameters of regression polynomial

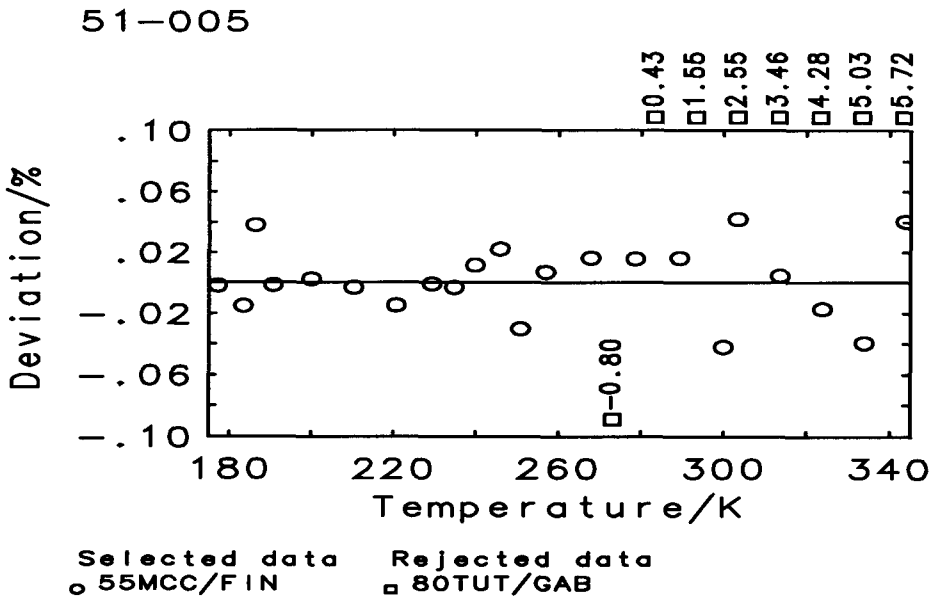
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	30	22	0.125	5.16-3	0.02	3.12-6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
177.2–343.8		2.53190+1	-7.86980	2.87769	-2.52948-1		II

TABLE 51.5.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} ($J K^{-1} g^{-1}$)	1.752	1.753	1.758	1.765	1.774	1.785	1.799
C_{sat} ($J K^{-1} mol^{-1}$)	158.0	158.1	158.5	159.1	160.0	161.0	162.2
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J K^{-1} g^{-1}$)	1.814	1.831	1.850	1.857	1.871	1.893	1.911
C_{sat} ($J K^{-1} mol^{-1}$)	163.6	165.2	166.9	167.4	168.7	170.7	172.4
Temp. (K)	300	310	320	330	340		
c_{sat} ($J K^{-1} g^{-1}$)	1.916	1.940	1.965	1.991	2.018		
C_{sat} ($J K^{-1} mol^{-1}$)	172.8	175.0	177.2	179.6	182.0		

TABLE 51.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	22	1.633	6.56–2	0.33	3.48–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
177.2–343.8	551.00	5.42924	5.05368	1.30825+1	1.45818		III



Name: 1,1'–Thiobisethane
Formula: $C_4H_{10}S$

CAS–RN: 352–93–2
Group No.: 51–006
Molar Mass: 90.19

TABLE 51.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52SCO/FIN1	182.0–316.1	26	0.20	99.995	melpt	C_{sat}	BSAO	43RUE/HUF
82TUT/GAB	273.0–373.0	eqn	0.40	99.77	chrom	C_p	BSAO	62KOL/SER

TABLE 51.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
52SCO/FIN1	182.0–316.1	26	0.20	0.095	3.84–3	0.02	2.13–6	1
				Rejected data				
82TUT/GAB	(2.19–1, 1.07, 1.05–1, 2)							

TABLE 51.6.3. Parameters of regression polynomial

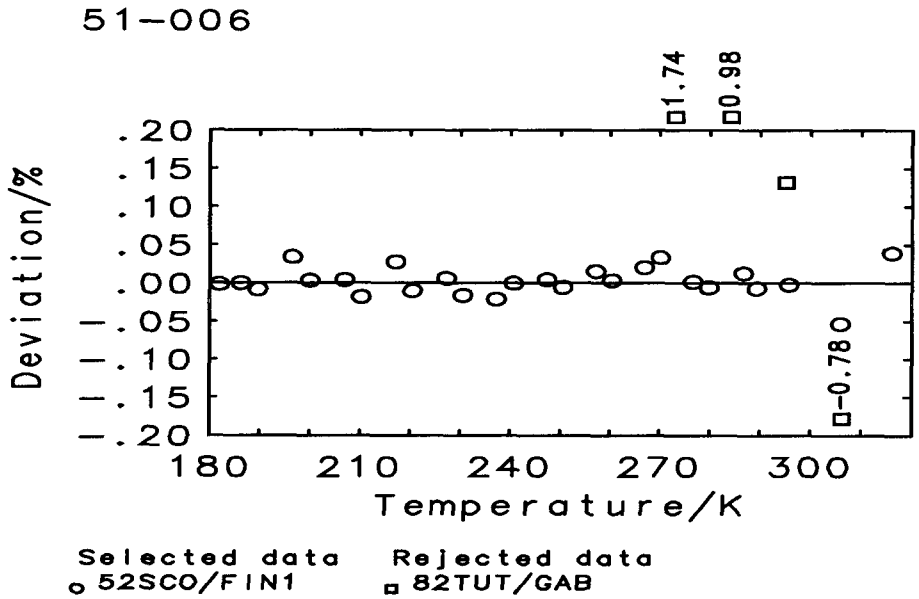
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	36	26	0.104	4.18–3	0.02	2.13–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
182.0–316.1		2.42561+1	–6.72456	2.41861	–1.91988–1		II

TABLE 51.6.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.739	1.742	1.747	1.754	1.763	1.774	1.788
C_{sat} (J K^{-1}mol^{-1})	156.9	157.1	157.5	158.2	159.0	160.0	161.3
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.803	1.821	1.839	1.846	1.860	1.882	1.901
C_{sat} (J K^{-1}mol^{-1})	162.6	164.2	165.9	166.5	167.7	169.7	171.4
Temp. (K)	300	310	320				
c_{sat} (J K^{-1}g^{-1})	1.905	1.930	1.956				
C_{sat} (J K^{-1}mol^{-1})	171.8	174.0	176.4				

TABLE 51.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	36	26	0.831	3.26–2	0.17	8.96–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
182.0–316.1	557.00	1.34440+1	8.50805	9.75487	5.31092		II



Name: 3,4–Dithiahexane
Formula: $C_4H_{10}S_2$

CAS–RN: 110–81–6
Group No.: 51–007
Molar Mass: 122.26

TABLE 51.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52SCO/FIN2	168.2–299.3	22	0.20	99.92	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.199	4.68–3	0.02	1.91–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
168.2–299.3		2.78189+1	–5.85871	2.07495	–1.60547–1		II

TABLE 51.7.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.569	1.568	1.569	1.572	1.576	1.582	1.589
C_{sat} (J K^{-1}mol^{-1})	191.8	191.7	191.9	192.2	192.7	193.4	194.3
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.598	1.607	1.618	1.630	1.634	1.643	1.657
C_{sat} (J K^{-1}mol^{-1})	195.3	196.5	197.8	199.3	199.8	200.9	202.6
Temp. (K)	298.15	300					
c_{sat} (J K^{-1}g^{-1})	1.669	1.672					
C_{sat} (J K^{-1}mol^{-1})	204.0	204.4					

TABLE 51.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	20	1.055	2.49–2	0.11	3.92–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
175.6–299.3	642.00	6.14274+1	2.84373+1	–5.56560	3.31723+1		II

Name: 1–(Ethylthio)propane
Formula: $C_5H_{12}S$

CAS–RN: 4110–50–3
Group No.: 51–008
Molar Mass: 104.22

TABLE 51.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61MCC/FIN	165.6–366.0	25	0.20	99.97	melpt	C_{sat}	BSAO	47HUF

TABLE 51.8.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.147	7.07–3	0.03	2.29–6	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
165.6–265.0		2.78739+1	–7.93320	2.94585	–2.46762–1		II
265.0–366.0		3.16566+1	–1.22155+1	4.56182	–4.50029–1		II

TABLE 51.8.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.730	1.731	1.735	1.741	1.749	1.759	1.772
C_{sat} (J K^{-1}mol^{-1})	180.3	180.4	180.8	181.4	182.3	183.3	184.7
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.786	1.803	1.821	1.841	1.847	1.862	1.884
C_{sat} (J K^{-1}mol^{-1})	186.2	187.9	189.8	191.8	192.5	194.1	196.4
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.904	1.908	1.932	1.957	1.983	2.008	2.034
C_{sat} (J K^{-1}mol^{-1})	198.4	198.8	201.4	204.0	206.6	209.3	211.9
Temp. (K)	360	370					
c_{sat} (J K^{-1}g^{-1})	2.059	2.083					
C_{sat} (J K^{-1}mol^{-1})	214.6	217.1					

TABLE 51.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	23	2.217	1.03–1	0.44	7.55–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
171.8–366.0	584.00	5.70547–1	4.01119	1.59849+1	2.02885–2		III

Name: 2–Methyl–2–(methylthio)propane
Formula: $C_5H_{12}S$

CAS–RN: 6163–64–0
Group No.: 51–009
Molar Mass: 104.22

TABLE 51.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62SCO/GOO	190.0–364.4	21	0.20	99.98	melpt	C_{sat}	BSAO	47HUF

TABLE 51.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.112	5.20–3	0.02	1.82–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
190.0–364.4		2.48364+1	–5.62605	2.41044	–2.05220–1		II

TABLE 51.9.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.711	1.722	1.735	1.750	1.767	1.786	1.805
C_{sat} (J·K^{-1}mol^{-1})	178.3	179.5	180.9	182.4	184.2	186.1	188.2
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.827	1.849	1.857	1.873	1.898	1.919	1.924
C_{sat} (J K^{-1}mol^{-1})	190.4	192.7	193.5	195.2	197.8	200.0	200.5
Temp. (K)	310	320	330	340	350	360	
c_{sat} (J K^{-1}g^{-1})	1.950	1.978	2.006	2.035	2.064	2.094	
C_{sat} (J K^{-1}mol^{-1})	203.3	206.1	209.1	212.1	215.1	218.2	

TABLE 51.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	1.113	5.24–2	0.22	1.93–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
190.0–364.4	566.00	–3.62673	1.79323	1.65479+1	1.83372		III

Name: 1–(Methylthio)butane
Formula: $C_5H_{12}S$

CAS–RN: 628–29–5
Group No.: 51–010
Molar Mass: 104.22

TABLE 51.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61MCC/FIN	186.9–358.0	23	0.20	99.96	melpt	C_{sat}	BSAO	47HUF

TABLE 51.10.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	0.096	4.37–3	0.02	1.58–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
186.9–270.0		3.04340+1	–1.05551+1	3.97267	–3.81658–1		II
270.0–358.0		2.74488+1	–7.23824	2.74420	–2.29994–1		II

TABLE 51.10.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.763	1.768	1.775	1.785	1.797	1.812	1.828
C_{sat} (J K^{-1}mol^{-1})	183.8	184.3	185.0	186.1	187.3	188.8	190.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.846	1.866	1.872	1.887	1.909	1.928	1.932
C_{sat} (J K^{-1}mol^{-1})	192.4	194.4	195.1	196.6	198.9	200.9	201.4
Temp. (K)	310	320	330	340	350	360	
c_{sat} (J K^{-1}g^{-1})	1.957	1.983	2.009	2.036	2.064	2.092	
C_{sat} (J K^{-1}mol^{-1})	204.0	206.6	209.4	212.2	215.1	218.1	

TABLE 51.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	23	23	1.559	7.34–2	0.31	3.74–4	3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
186.9–358.0	591.00	4.00770	5.85539	1.47529+1	6.85762–1		III

Name: 2–(Methylthio)butane
Formula: $C_5H_{12}S$

CAS–RN: 10359–64–5
Group No.: 51–011
Molar Mass: 104.22

TABLE 51.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80TUT/GAB	273.1–383.1	12S	0.40	not specified		C_p	BSAO	62KOL/SER

TABLE 51.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.064	6.40–3	0.03	–1.10–5	3
Temp. range K		A_1	A_2				Level of uncertainty
273.1–383.1		7.25435	4.75468				VI

TABLE 51.11.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1}g^{-1}$)	1.60	1.61	1.64	1.68	1.71	1.72	1.75
C_p ($J K^{-1}mol^{-1}$)	167	168	171	175	178	179	183
Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1}g^{-1}$)	1.79	1.83	1.87	1.91	1.94	1.98	2.02
C_p ($J K^{-1}mol^{-1}$)	187	191	195	199	203	207	211

Name: Tetrakis(methylthia)methane
Formula: $C_5H_{12}S$

CAS–RN: 6156–25–8
Group No.: 51–012
Molar Mass: 104.22

TABLE 51.12.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
43BAC/PER	338.65	1.423	nosp	99.75	melpt	C_p	BSIO	43BAC/PER

Name: Methylthiocyclopentane
Formula: $C_6H_{12}S$

CAS–RN: 7133–36–0
Group No.: 51–013
Molar Mass: 116.23

TABLE 51.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74MES/FIN	173.2–368.6	25	0.20	99.973	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.13.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	0.130	5.93–3	0.03	2.37–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
173.2–270.0		3.21220+1	–1.49411+1	5.76232	–5.88590–1		II
270.0–368.6		2.74836+1	–9.78732	3.85353	–3.52937–1		II

TABLE 51.13.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.465	1.464	1.466	1.472	1.481	1.493	1.508
C_{sat} (J K^{-1}mol^{-1})	170.3	170.2	170.4	171.1	172.2	173.6	175.3
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.525	1.544	1.565	1.588	1.596	1.613	1.638
C_{sat} (J K^{-1}mol^{-1})	177.2	179.5	182.0	184.6	185.5	187.4	190.4
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.660	1.665	1.693	1.721	1.750	1.780	1.810
C_{sat} (J K^{-1}mol^{-1})	192.9	193.5	196.7	200.0	203.4	206.9	210.4
Temp. (K)	360	370					
c_{sat} (J K^{-1}g^{-1})	1.840	1.871					
C_{sat} (J K^{-1}mol^{-1})	213.9	217.4					

Name: 2-(Methylthio)pentane
Formula: $C_6H_{14}S$

CAS-RN: 13286-91-4
Group No.: 51-014
Molar Mass: 118.24

TABLE 51.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80TUT/GAB	273.1–383.1	12S	0.40	not specified		C_p	BSAO	62KOL/SER

TABLE 51.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.000	1.21–6	0.00	–6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
273.1–383.1		7.49083	4.76276				VI

TABLE 51.14.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.43	1.44	1.46	1.50	1.53	1.53	1.56
C_p (J K^{-1}mol^{-1})	169	170	173	177	180	181	185
Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.60	1.63	1.67	1.70	1.73	1.77	1.80
C_p (J K^{-1}mol^{-1})	189	193	197	201	205	209	213

Name: 1,1'–Thiobispropane
Formula: $C_6H_{14}S$

CAS–RN: 111–47–7
Group No.: 51–015
Molar Mass: 118.24

TABLE 51.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
61MCC/FIN	173.7–315.0	19	0.20	99.96	melpt	C_{sat}	BSAO	47HUF
82TUT/GAB	273.0–373.0	eqn	0.40	99.81	chrom	C_p	BSAO	62KOL/SER

TABLE 51.15.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61MCC/FIN	173.7–315.0	19	0.20	0.078	4.05–3	0.02	9.03–7	2
				Rejected data				
82TUT/GAB	(1.72, 6.02, 1.69, 4)							

TABLE 51.15.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	29	19	0.091	4.71–3	0.02	9.03–7	2

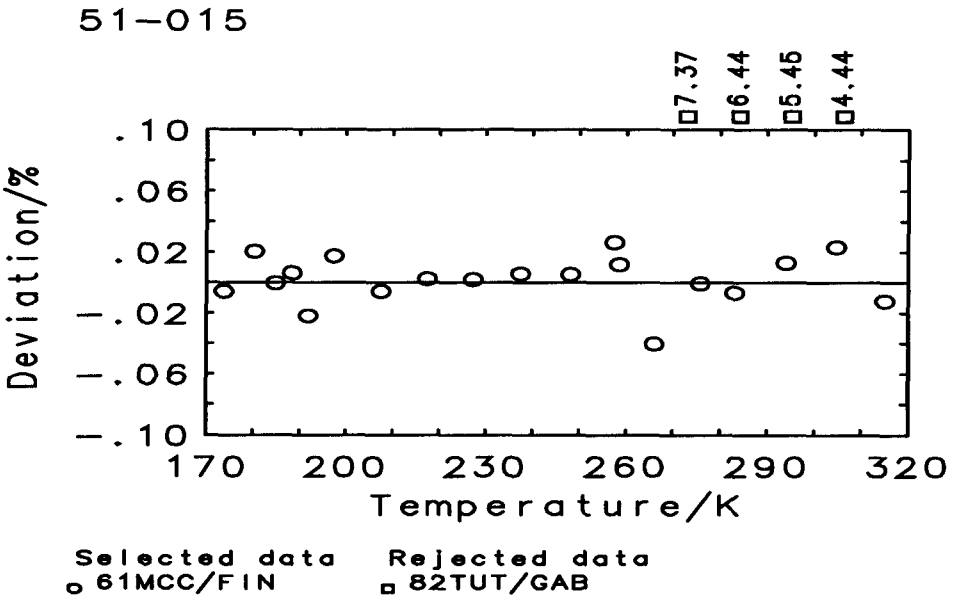
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
173.7–245.0	2.88160+1	–5.16301	1.53894	4.56495–3	II
245.0–315.0	3.96397+1	–1.84164+1	6.94851	–7.31431–1	II

TABLE 51.15.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} ($J K^{-1} g^{-1}$)	1.725	1.729	1.736	1.744	1.755	1.768	1.783
C_{sat} ($J K^{-1} mol^{-1}$)	204.0	204.5	205.2	206.2	207.5	209.0	210.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J K^{-1} g^{-1}$)	1.800	1.819	1.840	1.847	1.863	1.887	1.907
C_{sat} ($J K^{-1} mol^{-1}$)	212.8	215.1	217.6	218.4	220.3	223.1	225.4
Temp. (K)	300	310	320				
c_{sat} ($J K^{-1} g^{-1}$)	1.911	1.936	1.961				
C_{sat} ($J K^{-1} mol^{-1}$)	226.0	228.9	231.9				

TABLE 51.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	29	19	1.063	5.48–2	0.21	1.82–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
173.7–315.0	607.00	3.23869+1	1.91433+1	4.60742	1.36982+1		II



Name: 2,2'–Thiobispropane
Formula: $C_6H_{14}S$

CAS–RN: 625–80–9
Group No.: 51–016
Molar Mass: 118.24

TABLE 51.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67MES/TOD	N	203.7–383.2	30	0.70	99.992	melpt	C_{sat}	BSAO	47HUF

67MES/TOD error less than 0.2 % up to 250 K increasing to 0.7 % at 370 K

TABLE 51.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	30	30	0.042	7.88–3	0.03	4.51–6	2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
203.7–383.2		2.81735+1	–6.27383	2.89140	–2.73125–1		II

TABLE 51.16.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.758	1.773	1.790	1.808	1.828	1.849	1.871
C_{sat} (J K^{-1}mol^{-1})	207.9	209.7	211.7	213.8	216.1	218.6	221.2
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.894	1.902	1.918	1.943	1.964	1.969	1.995
C_{sat} (J K^{-1}mol^{-1})	224.0	224.9	226.8	229.8	232.2	232.8	235.9
Temp. (K)	320	330	340	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.022	2.049	2.077	2.104	2.132	2.159	2.187
C_{sat} (J K^{-1}mol^{-1})	239.1	242.3	245.5	248.8	252.1	255.3	258.6

TABLE 51.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.281	5.55–2	0.20	2.00–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
203.7–383.2	581.00	–4.74133	7.93615–1	1.92483+1	7.08160		II

Name: Dipropyl disulfide
Formula: $C_6H_{14}S_2$

CAS–RN: 629–19–6
Group No.: 51–017
Molar Mass: 150.31

TABLE 51.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
58HUB/DOU	193.6–351.2	20	0.20	99.97	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.209	1.32–2	0.04	9.92–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
193.6–351.2		3.87178+1	–1.16219+1	4.32351	–4.12203–1		II

TABLE 51.17.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.627	1.630	1.635	1.642	1.651	1.661	1.673
C_{sat} (J K^{-1}mol^{-1})	244.6	245.0	245.8	246.8	248.1	249.7	251.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.686	1.701	1.705	1.716	1.733	1.747	1.750
C_{sat} (J K^{-1}mol^{-1})	253.5	255.6	256.3	258.0	260.4	262.5	263.0
Temp. (K)	310	320	330	340	350		
c_{sat} (J K^{-1}g^{-1})	1.768	1.786	1.805	1.824	1.844		
C_{sat} (J K^{-1}mol^{-1})	265.7	268.5	271.3	274.2	277.1		

TABLE 51.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	1.008	6.32–2	0.20	2.06–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
193.6–351.2	674.00	1.43334+1	1.30442+1	1.47521+1	3.93748		II

Name: Methylthiobenzene
Formula: C_7H_8S

CAS–RN: 100–68–5
Group No.: 51–018
Molar Mass: 124.21

TABLE 51.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74MES/FIN	260.6–320.5	11	0.20	99.963	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 51.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.203	9.80–3	0.04	6.07–6	I
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
260.6–320.5		6.44222+1	–4.46849+1	1.56411+1	–1.71502		II

TABLE 51.18.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.595	1.609	1.614	1.626	1.643	1.659	1.662
C_{sat} (J K^{-1}mol^{-1})	198.2	199.9	200.5	201.9	204.1	206.0	206.5
Temp. (K)	310	320					
c_{sat} (J K^{-1}g^{-1})	1.681	1.700					
C_{sat} (J K^{-1}mol^{-1})	208.8	211.2					

Name: 2–(Methylthio)hexane
Formula: $C_7H_{16}S$

CAS–RN: 76858–84–9
Group No.: 51–019
Molar Mass: 132.27

TABLE 51.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80TUT/GAB	273.1–383.1	12S	0.40	not specified		C_p	BSAO	62KOL/SER

TABLE 51.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.000	1.21–6	0.00	–3.18–7	0

Temp. range K	A_1	A_2	Level of uncertainty
273.1–383.1	7.75303	4.76276	VI

TABLE 51.19.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.30	1.31	1.33	1.36	1.38	1.39	1.42
C_p ($J\,K^{-1}mol^{-1}$)	171	173	175	179	183	183	187
Temp. (K)	320	330	340	350	360	370	380
c_p ($J\,K^{-1}g^{-1}$)	1.45	1.48	1.51	1.54	1.57	1.60	1.63
C_p ($J\,K^{-1}mol^{-1}$)	191	195	199	203	207	211	215

Name: 2–(Methylthio)heptane
Formula: $C_8H_{18}S$

CAS–RN: 54063–12–6
Group No.: 51–020
Molar Mass: 146.30

TABLE 51.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80TUT/GAB	273.1–383.1	12S	0.40	not specified		C_p	BSAO	62KOL/SER

TABLE 51.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.022	2.17–3	0.01	–1.27–6	1
Temp. range K		A_1	A_2				Level of uncertainty
273.1–383.1		8.01275	4.76369				VI

TABLE 51.20.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	1.19	1.19	1.21	1.24	1.26	1.27	1.29
C_p (J K^{-1}mol^{-1})	174	175	178	181	185	185	189
Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	1.32	1.35	1.38	1.40	1.43	1.46	1.48
C_p (J K^{-1}mol^{-1})	193	197	201	205	209	213	217

Name: 1,1'–Thiobisbutane
Formula: $C_8H_{18}S$

CAS–RN: 544–40–1
Group No.: 51–021
Molar Mass: 146.30

TABLE 51.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61MCC/FIN	205.1–355.5	17	0.20	99.97	melpt	C_{sat}	BSAO	47HUF
82TUT/GAB	273.0–373.0	eqn	0.40	99.73	chrom	C_p	BSAO	62KOL/SER

TABLE 51.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61MCC/FIN	205.1–355.5	17	0.20	0.066	4.48–3	0.01	1.80–6	0
				Rejected data				
82TUT/GAB	(1.66, 4.60, 1.34, 6)							

TABLE 51.21.3. Parameters of cubic spline polynomials

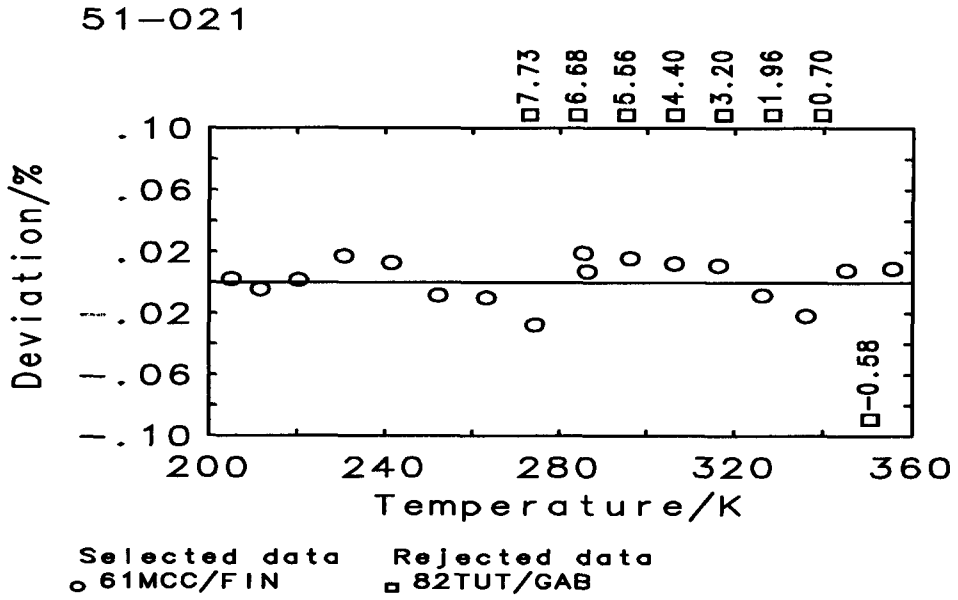
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	17	0.079	5.34–3	0.02	1.80–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
205.1–280.0		4.65824+1	–1.98176+1	7.54547	–7.68907–1		II
280.0–355.5		3.73535+1	–9.92946	4.01400	–3.48494–1		II

TABLE 51.21.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} ($J K^{-1} g^{-1}$)	1.769	1.780	1.794	1.810	1.829	1.850	1.872
C_{sat} ($J K^{-1} mol^{-1}$)	258.7	260.4	262.4	264.8	267.6	270.6	273.9
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} ($J K^{-1} g^{-1}$)	1.880	1.897	1.922	1.943	1.948	1.976	2.004
C_{sat} ($J K^{-1} mol^{-1}$)	275.0	277.5	281.2	284.3	285.0	289.1	293.2
Temp. (K)	330	340	350	360			
c_{sat} ($J K^{-1} g^{-1}$)	2.033	2.063	2.093	2.124			
C_{sat} ($J K^{-1} mol^{-1}$)	297.5	301.8	306.2	310.7			

TABLE 51.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	17	1.108	7.37–2	0.22	2.52–4	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
205.1–355.5	651.00	2.76497	9.97752	1.73405+1	1.91557–1		III



Name: 1,1'–Thiobispentane
Formula: $C_{10}H_{22}S$

CAS–RN: 872–10–6
Group No.: 51–022
Molar Mass: 174.35

TABLE 51.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.78	chrom	C_p	BSAO	62KOL/SER

TABLE 51.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	2.50–6	0.00	–3.82–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–372.9		4.16982+1	4.32984–1	1.06127–1			VI

TABLE 51.22.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	2.08	2.08	2.09	2.09	2.10	2.10	2.10
C_p ($J\,K^{-1}mol^{-1}$)	363	363	364	365	365	365	366
Temp. (K)	320	330	340	350	360	370	
c_p ($J\,K^{-1}g^{-1}$)	2.11	2.11	2.12	2.12	2.13	2.13	
C_p ($J\,K^{-1}mol^{-1}$)	367	368	369	370	371	372	

Name: 1,1'–Thiobisbenzene
Formula: $C_{12}H_{10}S$

CAS–RN: 139–66–2
Group No.: 51–023
Molar Mass: 186.28

TABLE 51.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
31SMI/AND2	259.8–298.5	4	nosp	97.5	estim	C_p	DSIO	26AND/LYN

TABLE 51.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.032	3.08–2	0.10	1.38–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
259.8–298.5		5.33881+1	–1.99256+1	4.34399			V

TABLE 51.23.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.38	1.40	1.40	1.41	1.43	1.45	1.46
C_p (J K^{-1}mol^{-1})	257	260	261	263	267	271	272

Name: 1,1'-Thiobishexane
Formula: $C_{12}H_{26}S$

CAS-RN: 6294-31-1
Group No.: 51-024
Molar Mass: 202.40

TABLE 51.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.57	chrom	C_p	BSAO	62KOL/SER

TABLE 51.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	3.53–6	0.00	–7.63–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–372.9		5.08763+1	4.66318–1	1.09101–1			VI

TABLE 51.24.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.17	2.18	2.18	2.18	2.19	2.19	2.19
C_p (J K^{-1}mol^{-1})	440	440	441	442	443	443	444
Temp. (K)	320	330	340	350	360	370	
c_p (J K^{-1}g^{-1})	2.20	2.20	2.21	2.21	2.22	2.22	
C_p (J K^{-1}mol^{-1})	445	446	447	448	449	450	

Name: 1,1'-Thiobisheptane
Formula: $C_{14}H_{30}S$

CAS-RN: 629-65-2
Group No.: 51-025
Molar Mass: 230.46

TABLE 51.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.63	chrom	C_p	BSAO	62KOL/SER

TABLE 51.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	3.53–6	0.00	1.53–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–372.9		5.78171+1	4.99884–1	1.11986–1			VI

TABLE 51.25.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.16	2.17	2.17	2.17	2.18	2.18	2.18
C_p (J K^{-1}mol^{-1})	499	499	500	501	501	502	503
Temp. (K)	320	330	340	350	360	370	
c_p (J K^{-1}g^{-1})	2.19	2.19	2.19	2.20	2.20	2.21	
C_p (J K^{-1}mol^{-1})	504	505	506	507	508	509	

Name: 1,1'–Thiobisoctane
Formula: $C_{16}H_{34}S$

CAS–RN: 2690–08–6
Group No.: 51–026
Molar Mass: 258.51

TABLE 51.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.7	chrom	C_p	BSAO	62KOL/SER

TABLE 51.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	4.99–6	0.00	–7.63–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–372.9		6.65295+1	4.99471–1	1.14982–1			VI

TABLE 51.26.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.21	2.21	2.21	2.22	2.22	2.22	2.23
C_p (J K^{-1}mol^{-1})	571	572	572	573	574	574	575
Temp. (K)	320	330	340	350	360	370	
c_p (J K^{-1}g^{-1})	2.23	2.23	2.24	2.24	2.25	2.25	
C_p (J K^{-1}mol^{-1})	576	577	578	579	581	582	

Name: 1,1'–Thiobisnonane
Formula: $C_{18}H_{38}S$

CAS–RN: 929–98–6
Group No.: 51–027
Molar Mass: 286.57

TABLE 51.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.89	chrom	C_p	BSAO	62KOL/SER

TABLE 51.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	6.45–6	0.00	–7.63–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–372.9		7.53524+1	5.32069–1	1.17851–1			VI

TABLE 51.27.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.25	2.25	2.26	2.26	2.26	2.26	2.27
C_p (J K^{-1}mol^{-1})	646	646	647	648	648	649	650
Temp. (K)	320	330	340	350	360	370	
c_p (J K^{-1}g^{-1})	2.27	2.27	2.28	2.28	2.29	2.29	
C_p (J K^{-1}mol^{-1})	651	652	653	654	655	656	

Name: 1,1'–Thiobisdecane
Formula: $C_{20}H_{42}S$

CAS–RN: 693–83–4
Group No.: 51–028
Molar Mass: 314.62

TABLE 51.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TUT/GAB	273.0–373.0	eqn	0.40	99.88	chrom	C_p	BSAO	62KOL/SER

TABLE 51.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	2.88–6	0.00	7.63–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–372.9		8.45148+1	5.65698–1	1.20743–1			VI

TABLE 51.28.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	2.30	2.30	2.30	2.30	2.31	2.31	2.31
C_p ($J\,K^{-1}mol^{-1}$)	723	723	724	725	726	726	727
Temp. (K)	320	330	340	350	360	370	
c_p ($J\,K^{-1}g^{-1}$)	2.31	2.32	2.32	2.32	2.33	2.33	
C_p ($J\,K^{-1}mol^{-1}$)	728	729	730	731	733	734	

52. Thiols

The thiol family contains measurements for 18 compounds, all of which were carried out all over a range of temperatures.

All measurements (except for methanethiol) were performed at BMB. These data have a reported uncertainty of 0.2 % and can be considered as highly reliable. The first member of the homologous series of alkanethiols, methanethiol, was investigated at CITP (42RUS/OSB) only and the data can be also regarded as very reliable.

The heat capacity curve $C_p = f(T)$ for alkanethiols with the number of carbon atoms below C_6 exhibits a clear minimum located several tens of kelvins above the triple point temperature. In such cases, the lower temperature limit of the quasipolynomial equation was shifted to this minimum. A detailed review and an attempt to explain the general behavior for different types of compounds can be found in the literature (93ZAB/BUR).

Name: Methanethiol
Formula: CH_4S

CAS-RN: 74-93-1
Group No.: 52-001
Molar Mass: 48.11

TABLE 52.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
42RUS/OSB	154.2–271.1	16	0.20	99.948	melpt	C_p	BSAO	41YOS/GAR

TABLE 52.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	16	16	0.352	7.43-3	0.07	9.00-6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
154.2–271.1		1.37932+1	-3.09881	7.11605-1			III

TABLE 52.1.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.857	1.842	1.829	1.818	1.810	1.805	1.802
C_p (J K^{-1}mol^{-1})	89.35	88.61	87.98	87.48	87.09	86.82	86.67
Temp. (K)	220	230	240	250	260	270	
c_p (J K^{-1}g^{-1})	1.801	1.803	1.807	1.814	1.823	1.834	
C_p (J K^{-1}mol^{-1})	86.64	86.72	86.93	87.25	87.69	88.25	

Name: Ethanethiol
Formula: C_2H_6S

CAS-RN: 75-08-1
Group No.: 52-002
Molar Mass: 62.14

TABLE 52.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
52MCC/SCO	130.1–315.3	27	0.20	99.978	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	27	0.291	7.93–3	0.06	7.45–6	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
130.1–315.3		1.62171+1	–2.83429	7.20314–1			II

TABLE 52.2.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J $K^{-1}g^{-1}$)	1.840	1.828	1.818	1.810	1.804	1.800	1.797
C_{sat} (J $K^{-1}mol^{-1}$)	114.3	113.6	113.0	112.5	112.1	111.8	111.7
Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J $K^{-1}g^{-1}$)	1.797	1.799	1.802	1.808	1.815	1.824	1.836
C_{sat} (J $K^{-1}mol^{-1}$)	111.7	111.8	112.0	112.3	112.8	113.4	114.1
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J $K^{-1}g^{-1}$)	1.849	1.853	1.864	1.881	1.896	1.900	1.921
C_{sat} (J $K^{-1}mol^{-1}$)	114.9	115.2	115.8	116.9	117.8	118.0	119.3
Temp. (K)	320						
c_{sat} (J $K^{-1}g^{-1}$)	1.943						
C_{sat} (J $K^{-1}mol^{-1}$)	120.8						

TABLE 52.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	15	0.403	1.12–2	0.08	1.33–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
207.9–315.3	499.00	3.97271	2.53442	1.05506+1	1.55681		II

Name: 1–Propanethiol
Formula: C_3H_8S

CAS–RN: 107–03–9
Group No.: 52–003
Molar Mass: 76.16

TABLE 52.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
56PEN/SCO	167.6–314.6	19	0.20	99.985	melpt	C_{sat}	BSAO	47HUF

TABLE 52.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.202	6.91–3	0.04	3.82–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
167.6–314.6		2.25592+1	–7.00308	2.31586	–1.84413–1		II

TABLE 52.3.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.795	1.788	1.785	1.784	1.786	1.790	1.797
C_{sat} (J K^{-1}mol^{-1})	136.7	136.2	135.9	135.9	136.0	136.3	136.9
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.806	1.817	1.830	1.845	1.850	1.862	1.881
C_{sat} (J K^{-1}mol^{-1})	137.5	138.4	139.4	140.5	140.9	141.8	143.3
Temp. (K)	298.15	300	310				
c_{sat} (J K^{-1}g^{-1})	1.897	1.901	1.923				
C_{sat} (J K^{-1}mol^{-1})	144.5	144.8	146.4				

TABLE 52.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	14	0.814	2.75–2	0.16	6.69–5	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
201.3–314.6	536.00	1.15064+1	6.15764	9.84120	5.37530		II

Name: 2–Propanethiol
Formula: C_3H_8S

CAS–RN: 75–33–2
Group No.: 52–004
Molar Mass: 76.16

TABLE 52.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
54MCC/FIN2	149.3–321.6	22	0.20	99.989	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.294	9.82–3	0.06	8.06–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
149.3–321.6		1.62505+1	–7.11558–1	1.87587–1	6.33198–2		II

TABLE 52.4.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J $K^{-1}g^{-1}$)	1.727	1.730	1.735	1.741	1.748	1.756	1.765
C_{sat} (J $K^{-1}mol^{-1}$)	131.5	131.8	132.2	132.6	133.1	133.7	134.4
Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J $K^{-1}g^{-1}$)	1.776	1.788	1.801	1.816	1.832	1.850	1.856
C_{sat} (J $K^{-1}mol^{-1}$)	135.3	136.2	137.2	138.3	139.5	140.9	141.3
Temp. (K)	280	290	298.15	300	310	320	
c_{sat} (J $K^{-1}g^{-1}$)	1.869	1.890	1.908	1.912	1.936	1.962	
C_{sat} (J $K^{-1}mol^{-1}$)	142.3	143.9	145.3	145.6	147.4	149.4	

TABLE 52.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	22	22	0.777	2.63–2	0.16	6.47–5	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
149.3–321.6	517.00	3.17831	3.24560	1.20695+1	7.78105–1		II

Name: 1–Butanethiol
Formula: $C_4H_{10}S$

CAS–RN: 109–79–5
Group No.: 52–005
Molar Mass: 90.19

TABLE 52.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
57SCO/FIN	160.2–314.3	20	0.20	99.99	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.181	7.23–3	0.04	4.86–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
160.2–314.3		2.94149+1	–1.15082+1	3.97637	–3.67382–1		II

TABLE 52.5.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.814	1.801	1.792	1.787	1.785	1.787	1.791
C_{sat} (J K^{-1}mol^{-1})	163.6	162.4	161.6	161.2	161.0	161.1	161.6
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.799	1.809	1.821	1.836	1.853	1.859	1.872
C_{sat} (J K^{-1}mol^{-1})	162.2	163.1	164.3	165.6	167.1	167.6	168.8
Temp. (K)	290	298.15	300	310			
c_{sat} (J K^{-1}g^{-1})	1.892	1.910	1.914	1.937			
C_{sat} (J K^{-1}mol^{-1})	170.6	172.2	172.6	174.7			

TABLE 52.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	13	1.011	4.04–2	0.20	1.21–4	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
200.3–314.3	569.00	2.43901+1	1.22200+1	6.74460	1.21702+1	II

Name: 2–Butanethiol
Formula: $C_4H_{10}S$

CAS–RN: 513–53–1
Group No.: 52–006
Molar Mass: 90.19

TABLE 52.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
58MCC/FIN	135.5–306.9	28	0.20	99.9	melpt	C_{sat}	BSAO	47HUF

TABLE 52.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.277	1.08–2	0.06	8.58–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
135.5–306.9		2.29105+1	–4.58247	1.43710	–5.38103–2		II

TABLE 52.6.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.767	1.760	1.755	1.752	1.752	1.754	1.757
C_{sat} (J K^{-1}mol^{-1})	159.3	158.7	158.3	158.1	158.0	158.2	158.5
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.763	1.771	1.781	1.793	1.806	1.822	1.840
C_{sat} (J K^{-1}mol^{-1})	159.0	159.7	160.6	161.7	162.9	164.3	165.9
Temp. (K)	273.15	280	290	298.15	300	310	
c_{sat} (J K^{-1}g^{-1})	1.846	1.859	1.880	1.899	1.903	1.928	
C_{sat} (J K^{-1}mol^{-1})	166.4	167.7	169.6	171.3	171.6	173.9	

TABLE 52.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	21	0.863	3.38–2	0.17	9.55–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
181.5–306.9	555.00	2.10391+1	1.09642+1	7.69431	1.00929+1		II

Name: 2–Methyl–1–propanethiol
Formula: $C_4H_{10}S$

CAS–RN: 513–44–0
Group No.: 52–007
Molar Mass: 90.19

TABLE 52.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
58SCO/MCC	137.4–348.8	24	0.20	99.993	melpt	C_{sat}	BSAO	47HUF

TABLE 52.7.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.188	7.40–3	0.04	4.13–6	3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
137.4–240.0		1.91865+1	1.32003–1	–6.03759–1	2.48593–1		II
240.0–348.8		2.78759+1	–1.07296+1	3.92192	–3.79973–1		II

TABLE 52.7.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.740	1.739	1.740	1.741	1.744	1.748	1.754
C_{sat} (J K^{-1}mol^{-1})	156.9	156.9	156.9	157.0	157.3	157.7	158.2
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.761	1.770	1.781	1.794	1.809	1.827	1.845
C_{sat} (J K^{-1}mol^{-1})	158.8	159.7	160.6	161.8	163.2	164.7	166.4
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.852	1.866	1.888	1.906	1.911	1.934	1.959
C_{sat} (J K^{-1}mol^{-1})	167.0	168.3	170.2	171.9	172.3	174.5	176.7
Temp. (K)	330	340	350				
c_{sat} (J K^{-1}g^{-1})	1.984	2.010	2.035				
C_{sat} (J K^{-1}mol^{-1})	179.0	181.2	183.5				

TABLE 52.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	21	1.754	7.02–2	0.35	3.99–4	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
169.3–348.8	557.00	3.29387	4.23943	1.36708+1	6.39803–1		III

Name: 2–Methyl–2–propanethiol
Formula: $C_4H_{10}S$

CAS–RN: 75–66–1
Group No.: 52–008
Molar Mass: 90.19

TABLE 52.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53MCC/SCO	280.9–329.1	12	0.20	99.989	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	12	12	0.141	5.87–3	0.03	3.50–6	0
Temp. range K		A_1	A_2				Level of uncertainty
280.9–329.1		1.36739+1	2.47679				II

TABLE 52.8.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.900	1.923	1.941	1.946	1.968	1.991	2.014
C_{sat} (J K^{-1}mol^{-1})	171.4	173.4	175.1	175.5	177.5	179.6	181.6

Name: Cyclopentanethiol
Formula: $C_5H_{10}S$

CAS–RN: 1679–07–8
Group No.: 52–009
Molar Mass: 102.20

TABLE 52.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
61BER/SCO	162.5–366.5	26	0.20	99.99	melpt	C_{sat}	BSAO	47HUF

TABLE 52.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	26	26	0.139	5.34–3	0.03	4.40–7	–4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
162.5–366.5	2.76550+1	–1.20403+1	4.39127	–4.11944–1	II

TABLE 52.9.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	1.460	1.452	1.449	1.449	1.452	1.458	1.467
C_{sat} (J K^{-1}mol^{-1})	149.2	148.4	148.1	148.0	148.4	149.0	149.9
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.479	1.493	1.510	1.529	1.550	1.557	1.572
C_{sat} (J K^{-1}mol^{-1})	151.2	152.6	154.3	156.3	158.4	159.1	160.7
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.596	1.617	1.622	1.648	1.675	1.703	1.732
C_{sat} (J K^{-1}mol^{-1})	163.1	165.2	165.7	168.4	171.2	174.1	177.0
Temp. (K)	350	360	370				
c_{sat} (J K^{-1}g^{-1})	1.761	1.790	1.819				
C_{sat} (J K^{-1}mol^{-1})	180.0	182.9	185.9				

TABLE 52.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	26	20	2.601	1.00–1	0.52	8.21–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
187.0–366.5	629.00	7.25271	8.30035	7.93675	1.58432		IV

Name: 2–Methyl–2–butanethiol
Formula: $C_5H_{12}S$

CAS–RN: 1679–09–0
Group No.: 52–010
Molar Mass: 104.22

TABLE 52.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62SCO/DOU	171.5–346.9	25	0.20	99.89	melpt	C_{sat}	BSAO	47HUF

TABLE 52.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	25	25	0.203	9.08–3	0.04	5.34–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
171.5–346.9		2.53029+1	–5.35364	2.09171	–1.54866–1		II

TABLE 52.10.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.714	1.719	1.725	1.733	1.743	1.755	1.769
C_{sat} (J K^{-1}mol^{-1})	178.6	179.1	179.8	180.6	181.7	182.9	184.3
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.784	1.801	1.819	1.839	1.845	1.860	1.882
C_{sat} (J K^{-1}mol^{-1})	185.9	187.7	189.6	191.6	192.3	193.8	196.2
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.901	1.906	1.930	1.956	1.983	2.010	2.038
C_{sat} (J K^{-1}mol^{-1})	198.1	198.6	201.2	203.8	206.6	209.5	212.4

TABLE 52.10.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	25	25	1.240	5.74–2	0.25	2.32–4	4

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
171.5–346.9	566.00	2.08364	4.62063	1.54513+1	2.34900–1	III

Name: 3–Methyl–1–butanethiol
Formula: $C_5H_{12}S$

CAS–RN: 541–31–1
Group No.: 52–011
Molar Mass: 104.22

TABLE 52.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74MES/FIN	140.5–370.6	28	0.20	99.95	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.123	5.64–3	0.02	3.13–6	–4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
140.5–370.6	2.90154+1	–9.63729	3.71294	–3.45666–1	II

TABLE 52.11.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_{sat} (J K^{-1}g^{-1})	1.743	1.735	1.730	1.728	1.730	1.734	1.741
C_{sat} (J K^{-1}mol^{-1})	181.7	180.8	180.3	180.1	180.3	180.7	181.5
Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.751	1.763	1.778	1.795	1.813	1.834	1.856
C_{sat} (J K^{-1}mol^{-1})	182.5	183.8	185.3	187.0	189.0	191.1	193.4
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.863	1.879	1.904	1.925	1.930	1.957	1.984
C_{sat} (J K^{-1}mol^{-1})	194.1	195.8	198.4	200.6	201.1	203.9	206.8
Temp. (K)	330	340	350	360	370		
c_{sat} (J K^{-1}g^{-1})	2.012	2.041	2.070	2.099	2.128		
C_{sat} (J K^{-1}mol^{-1})	209.7	212.7	215.7	218.8	221.8		

TABLE 52.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	20	1.821	8.57–2	0.36	5.06–4	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
187.0–370.6	604.00	–1.88900	3.62241	1.55243+1	2.46268–1		III

Name: 3–Methyl–2–butanethiol
Formula: $C_5H_{12}S$

CAS–RN: 2084–18–6
Group No.: 52–012
Molar Mass: 104.22

TABLE 52.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74MES/FIN	148.2–378.9	28	0.20	99.995	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.265	1.22–2	0.05	1.10–5	–5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
148.2–378.9		2.80233+1	–8.06622	3.00292	–2.53937–1		III

TABLE 52.12.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J K^{-1}g^{-1})	1.741	1.736	1.735	1.735	1.739	1.745	1.753
C_{sat} (J K^{-1}mol^{-1})	181.5	181.0	180.8	180.9	181.2	181.8	182.7
Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	1.764	1.776	1.791	1.808	1.826	1.846	1.853
C_{sat} (J K^{-1}mol^{-1})	183.8	185.1	186.7	188.4	190.3	192.4	193.1
Temp. (K)	280	290	298.15	300	310	320	330
c_{sat} (J K^{-1}g^{-1})	1.867	1.890	1.910	1.914	1.940	1.966	1.993
C_{sat} (J K^{-1}mol^{-1})	194.6	197.0	199.0	199.5	202.1	204.9	207.7
Temp. (K)	340	350	360	370	380		
c_{sat} (J K^{-1}g^{-1})	2.021	2.050	2.079	2.108	2.138		
C_{sat} (J K^{-1}mol^{-1})	210.6	213.6	216.6	219.7	222.8		

TABLE 52.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	25	2.845	1.34–1	0.57	1.26–3	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
165.2–378.9	584.50	1.66668	4.58871	1.56045+1	1.51339–1		IV

Name: 1–Pentanethiol
Formula: $C_5H_{12}S$

CAS–RN: 110–66–7
Group No.: 52–013
Molar Mass: 104.22

TABLE 52.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52FIN/SCO	200.3–321.0	28	0.20	99.94	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 52.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.331	1.54–2	0.07	1.66–5	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.3–321.0		3.07474+1	–9.71588	3.34207	–2.73838–1		II

TABLE 52.13.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.795	1.799	1.806	1.815	1.827	1.840	1.856
C_{sat} (J K^{-1}mol^{-1})	187.0	187.5	188.2	189.1	190.4	191.8	193.4
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.874	1.880	1.893	1.915	1.933	1.937	1.962
C_{sat} (J K^{-1}mol^{-1})	195.3	195.9	197.3	199.5	201.5	201.9	204.4
Temp. (K)	320						
c_{sat} (J K^{-1}g^{-1})	1.987						
C_{sat} (J K^{-1}mol^{-1})	207.1						

TABLE 52.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.720	3.40–2	0.14	8.30–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.3–321.0	598.00	2.64722+1	1.49111+1	6.88109	1.17493+1		II

Name: Benzenethiol
Formula: C_6H_6S

CAS–RN: 108–98–5
Group No.: 52–014
Molar Mass: 110.18

TABLE 52.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36PAR/TOD1	260.0–300.0	5S	0.70	not specified		C_p	BSIO	25PAR
56SCO/MCC2	262.5–374.5	15	0.20	99.98	melpt	C_{sat}	BSAO	47HUF

TABLE 52.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
56SCO/MCC2	262.5–374.5	15	0.20	0.067	2.85–3	0.01	–6.36–7	–2
				Rejected data				
36PAR/TOD1	(3.24–1, 1.54, 3.16–1, 4)							

TABLE 52.14.3. Parameters of regression polynomial

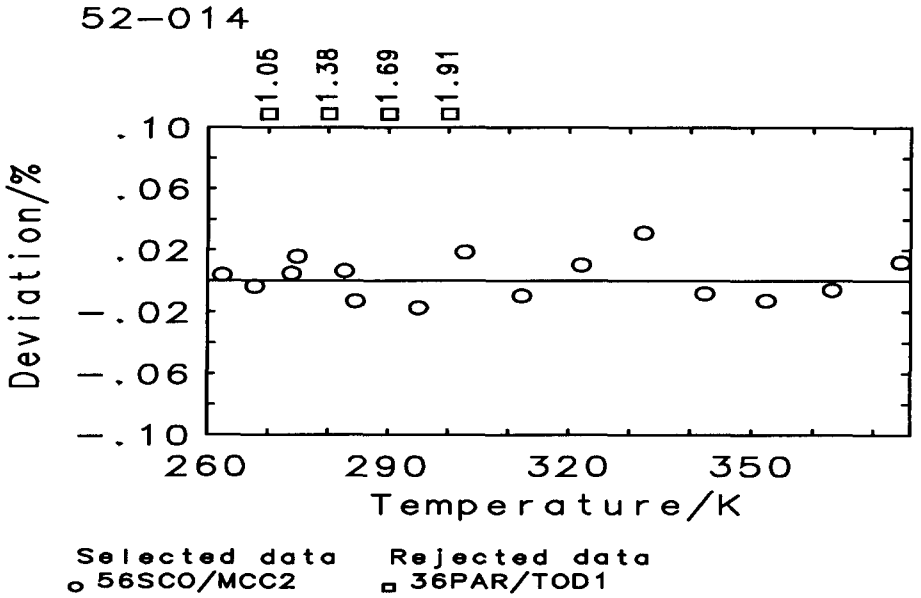
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	15	0.078	3.32–3	0.02	–6.36–7	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
262.5–374.5		2.27196+1	–4.70648	1.83088	–1.55734–1		II

TABLE 52.14.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} ($J K^{-1}g^{-1}$)	1.518	1.531	1.536	1.545	1.560	1.572	1.575
C_{sat} ($J K^{-1}mol^{-1}$)	167.3	168.7	169.2	170.3	171.9	173.2	173.6
Temp. (K)	310	320	330	340	350	360	370
c_{sat} ($J K^{-1}g^{-1}$)	1.591	1.608	1.625	1.642	1.660	1.678	1.697
C_{sat} ($J K^{-1}mol^{-1}$)	175.3	177.1	179.0	180.9	182.9	184.9	186.9

TABLE 52.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	15	0.208	8.77–3	0.04	6.74–6	0
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
262.5–374.5	685.00	–3.88114	1.40014	1.49752+1	2.68960		II



Name: Cyclohexanethiol
Formula: $C_6H_{12}S$

CAS–RN: 1569–69–3
Group No.: 52–015
Molar Mass: 116.23

TABLE 52.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67MES/TOD	N	196.6–365.3	21	0.70	99.978	melpt	C_{sat}	BSAO	47HUF

67MES/TOD error less than 0.2 % up to 250 K increasing to 0.7 % at 370 K

TABLE 52.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.059	9.13–3	0.04	6.36–6	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
196.6–365.3		2.83573+1	–1.00068+1	3.78972	–3.41428–1		II

TABLE 52.15.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.486	1.495	1.506	1.519	1.534	1.552	1.571
C_{sat} (J K^{-1}mol^{-1})	172.7	173.7	175.0	176.6	178.3	180.4	182.6
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.591	1.598	1.613	1.637	1.657	1.661	1.687
C_{sat} (J K^{-1}mol^{-1})	185.0	185.8	187.5	190.3	192.6	193.1	196.1
Temp. (K)	320	330	340	350	360	370	
c_{sat} (J K^{-1}g^{-1})	1.714	1.741	1.769	1.797	1.825	1.854	
C_{sat} (J K^{-1}mol^{-1})	199.2	202.3	205.6	208.8	212.2	215.5	

TABLE 52.15.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	21	21	0.416	6.64–2	0.29	3.06–4	3

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
196.6–365.3	664.00	4.11200	8.61869	9.70740	4.90461–1	IV

Name: 1-Hexanethiol
Formula: $C_6H_{14}S$

CAS-RN: 111-31-9
Group No.: 52-016
Molar Mass: 118.24

TABLE 52.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70FIN/MCC	200.3–371.9	20	0.20	99.978	melpt	C_{sat}	BSAO	47HUF

TABLE 52.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.215	1.20–2	0.04	7.92–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.3–371.9		4.23316+1	–1.85926+1	6.39874	–6.05128–1		II

TABLE 52.16.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.821	1.821	1.825	1.832	1.842	1.855	1.871
C_{sat} (J K^{-1}mol^{-1})	215.3	215.4	215.8	216.6	217.8	219.4	221.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.889	1.895	1.909	1.931	1.951	1.955	1.980
C_{sat} (J K^{-1}mol^{-1})	223.4	224.1	225.8	228.4	230.6	231.2	234.1
Temp. (K)	320	330	340	350	360	370	
c_{sat} (J K^{-1}g^{-1})	2.006	2.033	2.060	2.088	2.116	2.144	
C_{sat} (J K^{-1}mol^{-1})	237.2	240.4	243.6	246.9	250.2	253.5	

TABLE 52.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	2.125	1.16–1	0.43	7.96–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.3–371.9	620.00	8.92805	8.92904	1.52851+1	2.23177		III

Name: 1–Heptanethiol
Formula: $C_7H_{16}S$

CAS–RN: 1639–09–4
Group No.: 52–017
Molar Mass: 132.27

TABLE 52.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70FIN/MCC	232.1–359.4	16	0.20	99.97	melpt	C_{sat}	BSAO	47HUF

TABLE 52.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.386	2.33–2	0.08	2.35–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
232.1–359.4		3.24448+1	–4.59150	1.39699			II

TABLE 52.17.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	1.840	1.853	1.867	1.883	1.900	1.906	1.920
C_{sat} (J K^{-1}mol^{-1})	243.4	245.0	246.9	249.0	251.4	252.1	253.9
Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.941	1.960	1.964	1.989	2.015	2.043	2.073
C_{sat} (J K^{-1}mol^{-1})	256.7	259.2	259.8	263.0	266.5	270.3	274.2
Temp. (K)	350	360					
c_{sat} (J K^{-1}g^{-1})	2.105	2.139					
C_{sat} (J K^{-1}mol^{-1})	278.4	282.9					

TABLE 52.17.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.678	4.14–2	0.14	8.50–5	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
232.1–359.4	646.00	1.04369+1	1.17040+1	1.48259+1	2.32672		II

Name: 1–Decanethiol
Formula: $C_{10}H_{22}S$

CAS–RN: 143–10–2
Group No.: 52–018
Molar Mass: 174.35

TABLE 52.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70FIN/MCC	255.1–375.2	30	0.20	99.88	melpt	C_{sat}	BSAO	47HUF

TABLE 52.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.233	2.01–2	0.05	1.03–5	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
255.1–375.2		8.94719+1	–5.02033+1	1.60191+1	–1.51203		II

TABLE 52.18.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.939	1.952	1.957	1.970	1.990	2.008	2.013
C_{sat} (J K^{-1}mol^{-1})	338.0	340.4	341.3	343.4	346.9	350.2	350.9
Temp. (K)	310	320	330	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	2.038	2.065	2.094	2.124	2.154	2.184	2.214
C_{sat} (J K^{-1}mol^{-1})	355.4	360.1	365.1	370.3	375.5	380.8	386.1
Temp. (K)	380						
c_{sat} (J K^{-1}g^{-1})	2.244						
C_{sat} (J K^{-1}mol^{-1})	391.2						

TABLE 52.18.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.888	7.54–2	0.18	2.34–4	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
255.1–375.2	702.00	8.40907	1.55679+1	1.93022+1	1.13555		II

53. Heterocyclic Sulfur Compounds

This family contains 13 compounds all of which were measured over a range of temperatures.

The major part of the recommended values is based on measurements from BMB (49WAD/KNO, 52HUB/FIN, 53MCC/SUN, 53SCO/FIN, 54FIN/GRO, 54MCC/FIN1, 56PEN/FIN, 74MES/FIN) where 10 compounds were investigated and the results showed a reported uncertainty of 0.2 %. When establishing the recommended values, two recent measurements from NIPER (the BMB successor) (91CHI/KNI1, 91CHI/KNI2) have been included beside the earlier BMB values. This was the case for benzothiophene where the new data (91CHI/KNI2) allowed one to extend the recommended values close to the critical temperature. Similar treatment was given to the data for dibenzothiophene (91CHI/KNI1). In measuring both compounds, two different calorimeters were used, a classical adiabatic calorimeter (47HUF) up to 500 K (claimed error of 0.1 %), and at higher temperatures, a commercial Perkin-Elmer DSC-2 calorimeter (claimed error of 1 %) which was modified as described in the reference (89KNI/ARC). All auxiliary data for converting saturation heat capacities to isobaric heat capacities are available in the above two articles.

Dibenzothiophene was measured also at EREL (83ORO/MRA). The data agreed reasonably with the NIPER results within the reported uncertainty of measurement (1.5 %); however, they have not been included in the data correlation because the scatter of data was considered to be too high.

Three more compounds are part of this family: two compounds, 1,3- and 1,4-dithiane, were measured at SUU (83DEW/OFF) over a narrow temperature interval and the data obtained gave results with an estimated uncertainty around 1 % Highly reliable data for 2,5-dimethylthiophene were obtained at UMAA (65CAR/WES).

Name: Thietane
Formula: C_3H_6S

CAS–RN: 287–27–4
Group No.: 53–001
Molar Mass: 74.15

TABLE 53.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
53SCO/FIN	202.0–321.3	16	0.20	99.988	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 53.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.112	2.82–3	0.02	4.77–7	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
202.0–321.3		2.12015+1	–1.06987+1	3.92852	–4.00185–1		II

TABLE 53.1.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.381	1.385	1.392	1.403	1.415	1.430	1.447
C_{sat} (J K^{-1}mol^{-1})	102.4	102.7	103.2	104.0	104.9	106.1	107.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.466	1.473	1.487	1.509	1.527	1.531	1.555
C_{sat} (J K^{-1}mol^{-1})	108.7	109.2	110.2	111.9	113.2	113.6	115.3
Temp. (K)	320						
c_{sat} (J K^{-1}g^{-1})	1.579						
C_{sat} (J K^{-1}mol^{-1})	117.1						

TABLE 53.1.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	1.088	2.82–2	0.22	9.26–5	I
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
202.0–321.3	602.00	1.23903+1	8.36597	3.21486	4.58759		II

Name: Thiophene
Formula: C_4H_4S

CAS–RN: 110–02–1
Group No.: 53–002
Molar Mass: 84.14

TABLE 53.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
34JAC/PAR	237.8–289.3	9	nosp	not specified		C_p	BSIO	25PAR
49WAD/KNO	240.3–336.1	16	0.20	99.955	melpt	C_{sat}	BSAO	47HUF
85FIG/SZW	238.0–299.9	31	0.30	99.94	melpt	C_{sat}	BSAO	65SUG/SEK

TABLE 53.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
49WAD/KNO	240.3–336.1	16	0.20	2.057	5.99–2	0.41	4.90–2	12
85FIG/SZW	238.0–299.9	31	0.30	1.406	6.07–2	0.42	–5.58–2	–31
				Rejected data				
34JAC/PAR	(9.72–2, 0.66, 7.77–2, 6)							

TABLE 53.2.3. Parameters of regression polynomial

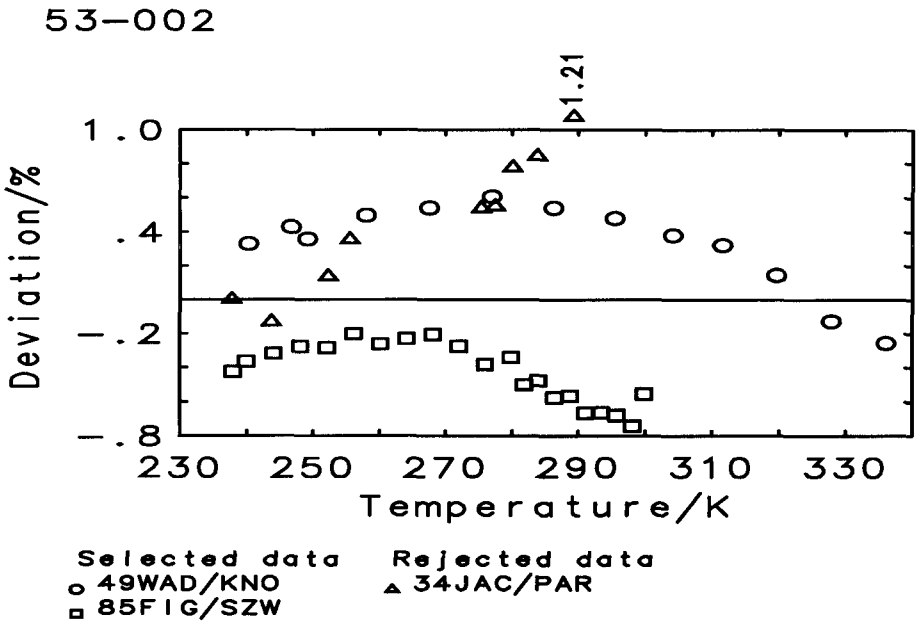
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	56	47	1.712	6.24–2	0.43	–2.01–2	–19
Temp. range K		A_1	A_2	A_3			Level of uncertainty
238.0–336.1		1.41351+1	–1.75177	6.65868–1			III

TABLE 53.2.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.360	1.375	1.391	1.409	1.415	1.428	1.448
C_{sat} (J K^{-1}mol^{-1})	114.5	115.7	117.1	118.6	119.0	120.1	121.8
Temp. (K)	298.15	300	310	320	330	340	
c_{sat} (J K^{-1}g^{-1})	1.466	1.470	1.492	1.517	1.542	1.569	
C_{sat} (J K^{-1}mol^{-1})	123.3	123.7	125.6	127.6	129.8	132.0	

TABLE 53.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	56	47	1.829	5.91–2	0.41	–7.94–4	–19
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
238.0–336.1	579.40	7.19476–1	3.36241	8.37738	3.84877–2		III



Name: Tetrahydrothiophene
Formula: C_4H_8S

CAS–RN: 110–01–0
Group No.: 53–003
Molar Mass: 88.17

TABLE 53.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
52HUB/FIN	180.2–333.4	24	0.20	99.987	melpt	C_{sat}	BSAO	47HUF

TABLE 53.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.204	6.42–3	0.04	2.86–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.2–333.4		2.05148+1	–8.47334	3.48919	–3.55066–1		II

TABLE 53.3.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	1.367	1.374	1.385	1.397	1.413	1.430	1.449
C_{sat} (J K^{-1}mol^{-1})	120.5	121.2	122.1	123.2	124.6	126.1	127.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.470	1.493	1.517	1.524	1.542	1.568	1.590
C_{sat} (J K^{-1}mol^{-1})	129.6	131.6	133.7	134.4	135.9	138.2	140.2
Temp. (K)	300	310	320	330			
c_{sat} (J K^{-1}g^{-1})	1.595	1.622	1.650	1.678			
C_{sat} (J K^{-1}mol^{-1})	140.6	143.0	145.5	147.9			

TABLE 53.3.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	1.411	4.50–2	0.28	2.06–4	4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
180.2–333.4	632.00	4.90483	7.51527	5.33250	8.00283–1		III

Name: 1,3–Dithiane
Formula: $C_4H_8S_2$

CAS–RN: 505–23–7
Group No.: 53–004
Molar Mass: 120.24

TABLE 53.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DEW/OFF	340.0–370.0	7S	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 53.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.796	1.68–1	0.80	1.94–3	3
Temp. range K		A_1	A_2				Level of uncertainty
340.0–370.0		6.67927	4.19447				V

TABLE 53.4.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.45	1.48	1.51	1.54
C_p ($J K^{-1} mol^{-1}$)	174	178	181	185

Name: 1,4–Dithiane
Formula: $C_4H_8S_2$

CAS–RN: 505–29–3
Group No.: 53–005
Molar Mass: 120.24

TABLE 53.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83DEW/OFF	390.0–400.0	3S	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 53.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.243	5.89–2	0.24	9.60–5	1

Temp. range K	A_1	A_2	Level of uncertainty
390.0–400.0	2.05137+1	9.60272–1	IV

TABLE 53.5.4. Recommended values of heat capacities

Temp. (K)	390	400
c_p ($J K^{-1} g^{-1}$)	1.677	1.684
C_p ($J K^{-1} mol^{-1}$)	201.7	202.5

Name: 2–Methylthiophene
Formula: C_5H_6S

CAS–RN: 554–14–3
Group No.: 53–006
Molar Mass: 98.17

TABLE 53.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56PEN/FIN	213.3–343.9	16	0.20	99.964	melpt	C_{sat}	BSAO	47HUF

TABLE 53.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.249	9.14–3	0.05	6.79–6	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
213.3–343.9		2.23550+1	–8.05917	3.14183	–3.10955–1		II

TABLE 53.6.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.390	1.399	1.411	1.424	1.439	1.455	1.472
C_{sat} (J K^{-1}mol^{-1})	136.4	137.4	138.5	139.8	141.2	142.8	144.5
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.478	1.490	1.509	1.526	1.529	1.550	1.571
C_{sat} (J K^{-1}mol^{-1})	145.1	146.3	148.2	149.8	150.1	152.2	154.2
Temp. (K)	330	340					
c_{sat} (J K^{-1}g^{-1})	1.592	1.614					
C_{sat} (J K^{-1}mol^{-1})	156.3	158.4					

TABLE 53.6.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	16	16	0.764	2.67–2	0.15	6.45–5	I
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
213.3–343.9	606.00	–2.12888	2.37270	1.16485+1	4.77529–1		II

Name: 3–Methylthiophene
Formula: C_5H_6S

CAS–RN: 616–44–4
Group No.: 53–007
Molar Mass: 98.17

TABLE 53.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53MCC/SUN	207.0–337.3	18	0.20	99.989	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 53.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.085	3.01–3	0.02	8.48–7	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
207.0–337.3		2.27761+1	–8.41867	3.26622	–3.24339–1		II

TABLE 53.7.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_{sat} (J K^{-1}g^{-1})	1.397	1.407	1.418	1.431	1.446	1.462	1.480
C_{sat} (J K^{-1}mol^{-1})	137.2	138.1	139.2	140.5	142.0	143.6	145.3
Temp. (K)	273.15	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.486	1.498	1.518	1.534	1.538	1.559	1.580
C_{sat} (J K^{-1}mol^{-1})	145.8	147.1	149.0	150.6	151.0	153.0	155.1
Temp. (K)	330	340					
c_{sat} (J K^{-1}g^{-1})	1.601	1.623					
C_{sat} (J K^{-1}mol^{-1})	157.2	159.3					

TABLE 53.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	0.740	2.58–2	0.15	6.07–5	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
207.0–337.3	610.00	–3.87492–2	3.72677	1.07687+1	1.00724–4		II

Name: 2–Methyltetrahydrothiophene
Formula: $C_5H_{10}S$

CAS–RN: 1795–09–1
Group No.: 53–008
Molar Mass: 102.20

TABLE 53.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74MES/FIN	168.0–389.0	28	0.20	99.76	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 53.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.219	9.24–3	0.04	3.68–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
168.0–389.0		2.14418+1	–6.79600	3.09194	–3.02280–1		II

TABLE 53.8.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_{sat} (J K^{-1}g^{-1})	1.411	1.421	1.433	1.448	1.465	1.484	1.504
C_{sat} (J K^{-1}mol^{-1})	144.2	145.2	146.5	148.0	149.7	151.6	153.7
Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.526	1.550	1.575	1.601	1.610	1.629	1.657
C_{sat} (J K^{-1}mol^{-1})	156.0	158.4	161.0	163.7	164.5	166.4	169.3
Temp. (K)	298.15	300	310	320	330	340	350
c_{sat} (J K^{-1}g^{-1})	1.680	1.686	1.715	1.745	1.775	1.806	1.836
C_{sat} (J K^{-1}mol^{-1})	171.7	172.3	175.3	178.4	181.4	184.6	187.7
Temp. (K)	360	370	380	390			
c_{sat} (J K^{-1}g^{-1})	1.867	1.897	1.926	1.955			
C_{sat} (J K^{-1}mol^{-1})	190.8	193.8	196.9	199.8			

TABLE 53.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	28	28	0.621	2.49–2	0.12	3.24–5	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
168.0–389.0	631.00	2.27808+2	2.14894+1	–4.86750	2.07168+2	7.74579+1	1.45011+2	II

Name: 3–Methyltetrahydrothiophene
Formula: $C_5H_{10}S$

CAS–RN: 4740–00–5
Group No.: 53–009
Molar Mass: 102.20

TABLE 53.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74MES/FIN	194.3–336.7	24	0.20	99.944	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 53.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.136	5.16–3	0.03	5.56–7	–1
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
194.3–336.7	2.20571+1	–7.34740	3.26574	–3.21256–1	II

TABLE 53.9.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_{sat} (J K^{-1}g^{-1})	1.453	1.469	1.487	1.507	1.529	1.552	1.577
C_{sat} (J K^{-1}mol^{-1})	148.5	150.1	152.0	154.0	156.3	158.6	161.2
Temp. (K)	270	273.15	280	290	298.15	300	310
c_{sat} (J K^{-1}g^{-1})	1.603	1.611	1.630	1.658	1.681	1.687	1.716
C_{sat} (J K^{-1}mol^{-1})	163.8	164.7	166.6	169.4	171.8	172.4	175.4
Temp. (K)	320	330	340				
c_{sat} (J K^{-1}g^{-1})	1.746	1.776	1.806				
C_{sat} (J K^{-1}mol^{-1})	178.4	181.5	184.6				

TABLE 53.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	24	24	0.824	3.22–2	0.16	8.66–5	2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
194.3–336.7	641.00	–2.64179	4.99248	9.48275	3.49478–1		II

Name: Tetrahydro–2*H*–thiopyran
Formula: $C_5H_{10}S$

CAS–RN: 1613–51–0
Group No.: 53–010
Molar Mass: 102.20

TABLE 53.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
54MCC/FIN1	295.6–341.5	9	0.20	99.986	melpt	C_{sat}	BSAO	43RUE/HUF

TABLE 53.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.521	1.05–2	0.05	7.42–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
295.6–341.5		7.94670	3.87960	1.40353–2			II

TABLE 53.10.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	1.604	1.636	1.668	1.700	1.733
C_{sat} (J K^{-1}mol^{-1})	163.9	167.2	170.5	173.8	177.1

Name: 2,5–Dimethylthiophene
Formula: C_6H_8S

CAS–RN: 638–02–8
Group No.: 53–011
Molar Mass: 112.20

TABLE 53.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65CAR/WES2	217.2–304.5	11	0.10	99.922	melpt	C_{sat}	BSAO	68WES/FUR

TABLE 53.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.868	1.79–2	0.09	2.24–5	2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
217.2–304.5	1.96226+1	–1.32433	6.49169–1	II

TABLE 53.11.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	1.471	1.483	1.496	1.510	1.524	1.540	1.545
C_{sat} (J K^{-1}mol^{-1})	165.1	166.4	167.8	169.4	171.0	172.8	173.3
Temp. (K)	280	290	298.15	300			
c_{sat} (J K^{-1}g^{-1})	1.557	1.574	1.589	1.593			
C_{sat} (J K^{-1}mol^{-1})	174.6	176.6	178.3	178.7			

TABLE 53.11.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.909	1.87–2	0.09	2.38–5	0

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
217.2–304.5	627.00	2.49929	5.72005	1.20215+1	2.73006–1	II

Name: Benzo[*b*]thiophene
Formula: C_8H_6S

CAS–RN: 95–15–8
Group No.: 53–012
Molar Mass: 134.20

TABLE 53.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54FIN/GRO1	307.8–329.7	5	0.20	99.968	melpt	C_{sat}	BSAO	47HUF
91CHI/KNI2	314.2–495.4	16	0.10	99.92	melpt	C_{sat}	BSAO	47HUF
91CHI/KNI2	300.0–750.0	24	1.00	99.92	melpt	C_{sat}	BDHT	89KNI/ARC

TABLE 53.12.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54FIN/GRO1	307.8–329.7	5	0.20	0.919	4.31–2	0.18	–4.03–2	–5
91CHI/KNI2	314.2–495.4	16	0.10	0.313	7.58–3	0.03	3.13–3	3
91CHI/KNI2	300.0–750.0	24	1.00	0.588	2.77–1	0.59	6.40–3	5

TABLE 53.12.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	45	0.601	2.18–1	0.47	4.56–5	3
C_{sat}	45	45	0.471	1.14–1	0.28	–1.07–4	5

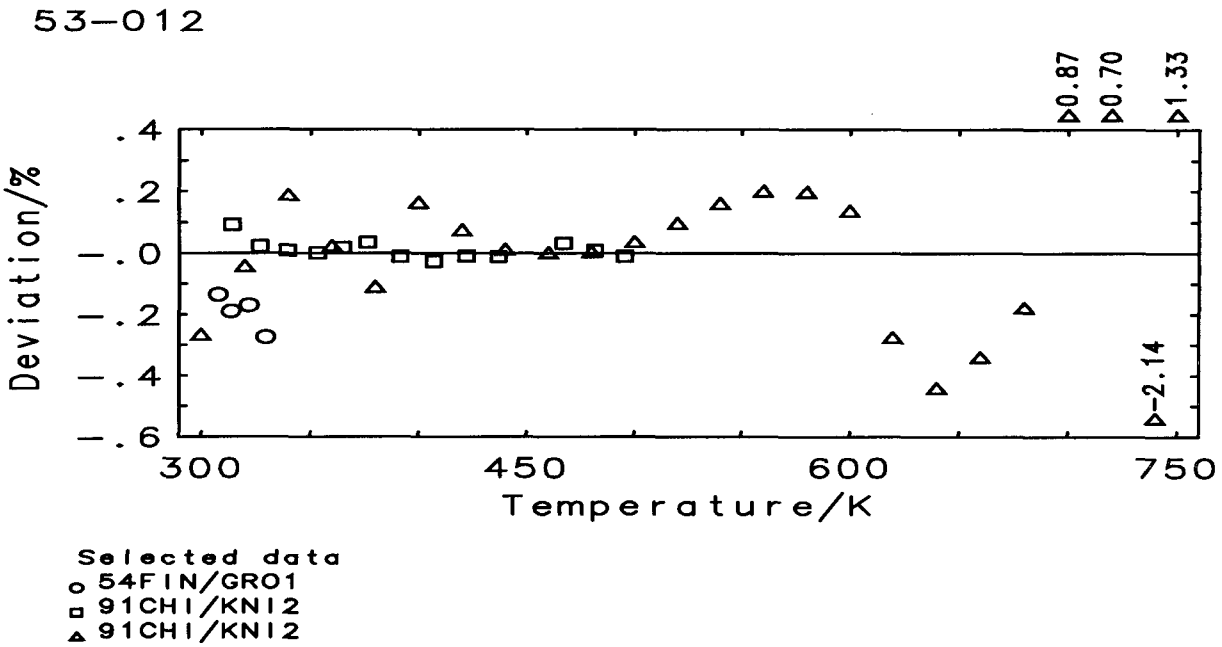
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
300.0–500.0	1.09070+1	4.04731	–3.38850–2	–3.06330–3	II
500.0–690.0	–1.66827+1	2.06012+1	–3.34466	2.17655–1	IV
690.0–750.0	–1.98052+4	8.62431+3	–1.25026+3	6.04551+1	V
300.0–500.0	1.10117+1	3.93798	2.59212–3	–6.98419–3	II
500.0–690.0	–2.96745	1.23255+1	–1.67490	1.04849–1	IV
690.0–750.0	–1.10695+4	4.82384+3	–6.98996+2	3.37919+1	V

TABLE 53.12.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p (J K^{-1}g^{-1})	1.404	1.427	1.450	1.474	1.497	1.520	1.542
C_p (J K^{-1}mol^{-1})	188.4	191.5	194.7	197.8	200.8	203.9	207.0
c_{sat} (J K^{-1}g^{-1})	1.404	1.427	1.450	1.474	1.497	1.520	1.542
C_{sat} (J K^{-1}mol^{-1})	188.4	191.5	194.7	197.8	200.8	203.9	207.0
Temp. (K)	370	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	1.565	1.588	1.610	1.633	1.655	1.678	1.700
C_p (J K^{-1}mol^{-1})	210.0	213.1	216.1	219.2	222.2	225.2	228.2
c_{sat} (J K^{-1}g^{-1})	1.565	1.588	1.611	1.633	1.655	1.678	1.700
C_{sat} (J K^{-1}mol^{-1})	210.1	213.1	216.1	219.2	222.2	225.2	228.1
Temp. (K)	440	450	460	470	480	490	500
c_p (J K^{-1}g^{-1})	1.722	1.744	1.766	1.788	1.810	1.832	1.853
C_p (J K^{-1}mol^{-1})	231.1	234.1	237.0	240.0	242.9	245.8	248.7
c_{sat} (J K^{-1}g^{-1})	1.722	1.744	1.766	1.788	1.809	1.831	1.852
C_{sat} (J K^{-1}mol^{-1})	231.1	234.0	237.0	239.9	242.8	245.7	248.5
Temp. (K)	510	520	530	540	550	560	570
c_p (J K^{-1}g^{-1})	1.875	1.896	1.918	1.940	1.962	1.984	2.006
C_p (J K^{-1}mol^{-1})	251.6	254.5	257.4	260.3	263.2	266.2	269.3
c_{sat} (J K^{-1}g^{-1})	1.873	1.894	1.916	1.937	1.958	1.979	2.000
C_{sat} (J K^{-1}mol^{-1})	251.4	254.2	257.1	259.9	262.7	265.6	268.5
Temp. (K)	580	590	600	610	620	630	640
c_p (J K^{-1}g^{-1})	2.029	2.053	2.077	2.102	2.128	2.155	2.182
C_p (J K^{-1}mol^{-1})	272.4	275.5	278.8	282.1	285.6	289.2	292.9
c_{sat} (J K^{-1}g^{-1})	2.022	2.043	2.065	2.087	2.110	2.133	2.156
C_{sat} (J K^{-1}mol^{-1})	271.3	274.2	277.2	280.1	283.2	286.2	289.3
Temp. (K)	650	660	670	680	690	700	710
c_p (J K^{-1}g^{-1})	2.211	2.241	2.272	2.304	2.337	2.38	2.44
C_p (J K^{-1}mol^{-1})	296.7	300.7	304.9	309.2	313.7	319	327
c_{sat} (J K^{-1}g^{-1})	2.179	2.203	2.228	2.253	2.279	2.31	2.35
C_{sat} (J K^{-1}mol^{-1})	292.5	295.7	299.0	302.4	305.8	310	315
Temp. (K)	720	730	740	750			
c_p (J K^{-1}g^{-1})	2.55	2.73	2.99	3.38			
C_p (J K^{-1}mol^{-1})	342	366	402	453			
c_{sat} (J K^{-1}g^{-1})	2.42	2.52	2.68	2.90			
C_{sat} (J K^{-1}mol^{-1})	324	338	359	389			

TABLE 53.12.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	45	45	1.100	1.29–1	0.36	2.24–2	1 1
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
300.0–750.0	764.00	–2.27107	2.76404–1	7.62773	4.32713+1	–2.54932+1	5.55789	IV



Name: Dibenzothiophene
Formula: $C_{12}H_8S$

CAS–RN: 132–65–0
Group No.: 53–013
Molar Mass: 184.26

TABLE 53.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83ORO/MRA	380.0–550.0	24S	1.50	99.9	chrom	C_p	BDHT	69PER/COM
91CHI/KNI1	377.2–515.7	16	0.10	99.986	melpt	C_{sat}	BSAO	47HUF
91CHI/KNI1	380.0–860.0	25	1.00	99.986	melpt	C_{sat}	BDHT	89KNI/ARC

TABLE 53.13.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
91CHI/KNI1	377.2–515.8	16	0.10	0.174	6.88–3	0.02	–8.51–5	–1
91CHI/KNI1	380.0–860.0	25	1.00	0.099	4.96–2	0.10	5.67–3	3
				Rejected data				
83ORO/MRA	(4.24–1, 1.21,–2.55–1, –12)							

TABLE 53.13.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	65	41	0.144	4.22–2	0.08	3.42–3	2
C_{sat}	65	41	0.135	2.76–2	0.06	2.04–3	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
377.2–520.0	9.06300	8.49276	–5.72539–1	2.53651–2	II
520.0–780.0	1.03521+1	7.74904	–4.29516–1	1.61970–2	IV
780.0–860.0	–3.41510+3	1.32523+3	–1.69337+2	7.23448	IV
377.2–520.0	8.35689	8.97523	–6.81722–1	3.35480–2	II
520.0–780.0	1.64694+1	4.29495	2.18332–1	–2.41478–2	IV
780.0–860.0	–1.62307+3	6.34889+2	–8.06270+1	3.43078	IV

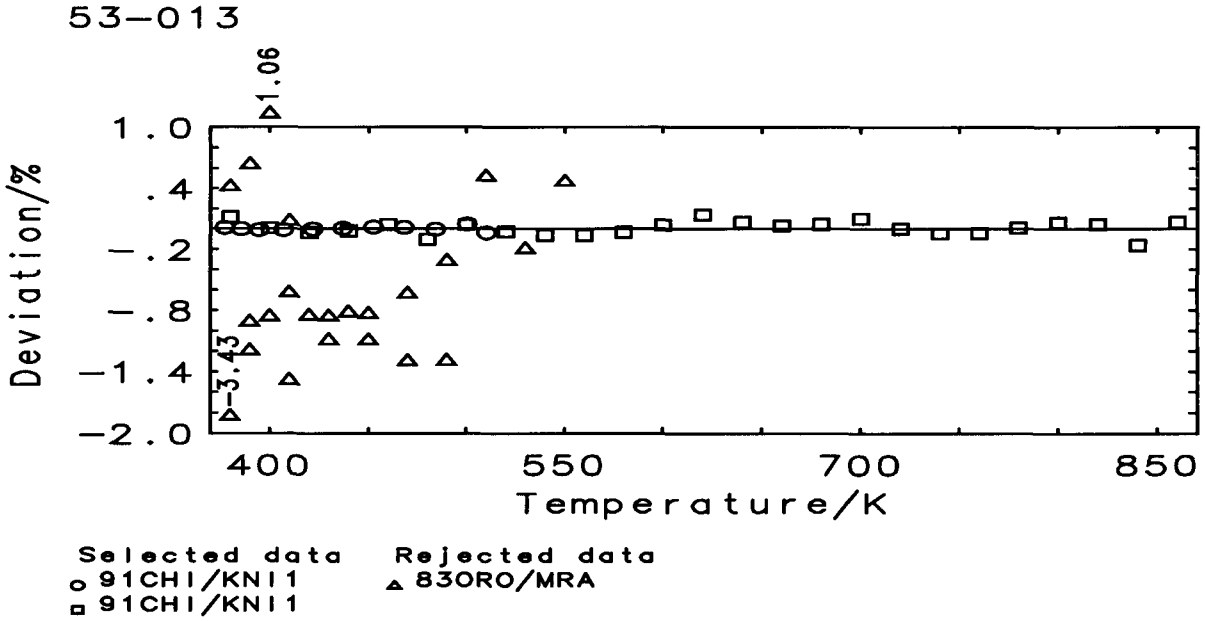
TABLE 53.13.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430	440
c_p ($J\,K^{-1}g^{-1}$)	1.555	1.578	1.602	1.625	1.648	1.670	1.692
C_p ($J\,K^{-1}mol^{-1}$)	286.5	290.9	295.1	299.4	303.6	307.7	311.9
c_{sat} ($J\,K^{-1}g^{-1}$)	1.555	1.578	1.602	1.625	1.648	1.670	1.692
C_{sat} ($J\,K^{-1}mol^{-1}$)	286.5	290.9	295.1	299.4	303.6	307.7	311.9
Temp. (K)	450	460	470	480	490	500	510
c_p ($J\,K^{-1}g^{-1}$)	1.715	1.737	1.758	1.780	1.801	1.822	1.843
C_p ($J\,K^{-1}mol^{-1}$)	315.9	320.0	324.0	327.9	331.9	335.8	339.6
c_{sat} ($J\,K^{-1}g^{-1}$)	1.715	1.736	1.758	1.780	1.801	1.822	1.843
C_{sat} ($J\,K^{-1}mol^{-1}$)	315.9	320.0	324.0	327.9	331.9	335.8	339.6
Temp. (K)	520	530	540	550	560	570	580
c_p ($J\,K^{-1}g^{-1}$)	1.864	1.885	1.905	1.926	1.946	1.966	1.986
C_p ($J\,K^{-1}mol^{-1}$)	343.5	347.3	351.1	354.8	358.5	362.2	365.9
c_{sat} ($J\,K^{-1}g^{-1}$)	1.864	1.885	1.905	1.926	1.946	1.966	1.986
C_{sat} ($J\,K^{-1}mol^{-1}$)	343.5	347.3	351.1	354.9	358.6	362.3	365.9
Temp. (K)	590	600	610	620	630	640	650
c_p ($J\,K^{-1}g^{-1}$)	2.006	2.025	2.045	2.064	2.084	2.103	2.122
C_p ($J\,K^{-1}mol^{-1}$)	369.6	373.2	376.8	380.4	383.9	387.4	391.0
c_{sat} ($J\,K^{-1}g^{-1}$)	2.006	2.025	2.045	2.064	2.083	2.101	2.120
C_{sat} ($J\,K^{-1}mol^{-1}$)	369.6	373.2	376.7	380.3	383.8	387.2	390.6
Temp. (K)	660	670	680	690	700	710	720
c_p ($J\,K^{-1}g^{-1}$)	2.141	2.160	2.178	2.197	2.216	2.234	2.253
C_p ($J\,K^{-1}mol^{-1}$)	394.5	397.9	401.4	404.9	408.3	411.7	415.1
c_{sat} ($J\,K^{-1}g^{-1}$)	2.138	2.156	2.174	2.191	2.209	2.226	2.243
C_{sat} ($J\,K^{-1}mol^{-1}$)	394.0	397.3	400.6	403.8	407.0	410.1	413.2
Temp. (K)	730	740	750	760	770	780	790
c_p ($J\,K^{-1}g^{-1}$)	2.271	2.289	2.308	2.326	2.344	2.362	2.381
C_p ($J\,K^{-1}mol^{-1}$)	418.5	421.9	425.2	428.6	431.9	435.3	438.6
c_{sat} ($J\,K^{-1}g^{-1}$)	2.259	2.275	2.291	2.307	2.322	2.337	2.352
C_{sat} ($J\,K^{-1}mol^{-1}$)	416.3	419.2	422.2	425.1	427.9	430.6	433.4
Temp. (K)	800	810	820	830	840	850	860
c_p ($J\,K^{-1}g^{-1}$)	2.401	2.425	2.455	2.493	2.540	2.600	2.672
C_p ($J\,K^{-1}mol^{-1}$)	442.4	446.8	452.4	459.3	468.1	479.0	492.4
c_{sat} ($J\,K^{-1}g^{-1}$)	2.367	2.384	2.404	2.427	2.454	2.487	2.525
C_{sat} ($J\,K^{-1}mol^{-1}$)	436.2	439.4	443.0	447.2	452.2	458.2	465.3

TABLE 53.13.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/−
C_p	65	41	0.372	1.61–1	0.30	1.68–2	6

Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
377.2–860.0	897.00	−2.36624	1.02086–1	9.22135	7.06493+1	−3.72753+1	6.83560	IV



61. Compounds of Carbon, Hydrogen, Halogen and Oxygen

This family contains 46 compounds, 6 of which have data at one temperature only.

For 28 compounds, measurements were carried out in the last century (*77BER, *81VON, *84WER, *87SCH, *95PIC) or soon after the beginning of the 20th century (02LOU2, 08BOG/WIN) and most of them have never been remeasured since. It is very difficult to estimate the uncertainty for all these data; all measurements were carried out using drop calorimeters and only average heat capacities were provided. In addition, the reported data lack any indication of the purity of the compounds used. For this reason, the recommended data have been assigned a high level of uncertainty.

For the three isomers of chlorobenzoic acid, the only measurements available in the literature were performed at YUNH (26AND/LYN) and published as parameters of a linear equation. For three compounds, hexafluoroacetone, oxalyl fluoride and trifluoroacetyl fluoride, measurements were carried out at WRUC (67PLA/PAC, 71HOD, 72PAC/HOD) and the resulting data showed a low uncertainty of around 0.2 %. The first and the last of these compounds exhibit an unusual variation of heat capacity with temperature. For trifluoroacetyl fluoride the heat capacity first rises from the triple point (113.69 K) reaching maximum around 150 K and then drops to a minimum at 189 K and again raises as the normal boiling temperature (214.1 K) is approached (which is the upper temperature limit of data from WRUC). Hexafluoroacetone (67PLA/PAC) exhibits a distinct minimum 45 K above the melting temperature.

Pentafluorophenol was investigated at NPLT (68AND/CON1) and at the same time at IICN (69PAU/LAV2); agreement of both data sets is good but the former source was preferred due to a smaller claimed error. This compound also exhibits a minimum on the $C_p = f(T)$ curve located 50 K above the melting temperature.

Name: Ethanedioyl difluoride
Formula: $C_2F_2O_2$

CAS-RN: 359-40-0
Group No.: 61-001
Molar Mass: 94.02

TABLE 61.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71HOD	262.4–271.1	7	nosp	99.94	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 61.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	0.313	1.81–2	0.09	2.42–5	0

Temp. range K	A_1	A_2	Level of uncertainty
262.4–271.1	1.53292+1	1.48258	III

TABLE 61.1.4. Recommended values of heat capacities

Temp. (K)	262	265	268	271
c_{sat} (J K^{-1}g^{-1})	1.699	1.703	1.707	1.711
C_{sat} (J K^{-1}mol^{-1})	159.8	160.1	160.5	160.9

Name: Trifluoroacetyl fluoride
Formula: C_2F_4O

CAS-RN: 354-34-7
Group No.: 61-002
Molar Mass: 116.02

TABLE 61.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72PAC/HOD	115.8–214.9	41	nosp	99.971	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 61.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	41	41	0.921	4.59-2	0.28	2.28-4	-3

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
115.8–214.9	2.93810	2.51580+1	-1.52648+1	3.04492	III

TABLE 61.2.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_{sat} (J $K^{-1}g^{-1}$)	1.176	1.185	1.189	1.190	1.189	1.186	1.184
C_{sat} (J $K^{-1}mol^{-1}$)	136.4	137.5	138.0	138.1	137.9	137.6	137.4

Temp. (K)	190	200	210
c_{sat} (J $K^{-1}g^{-1}$)	1.184	1.186	1.193
C_{sat} (J $K^{-1}mol^{-1}$)	137.3	137.6	138.4

Name: Trichloroacetaldehyde
Formula: C_2HCl_3O

CAS-RN: 75-87-6
Group No.: 61-003
Molar Mass: 147.39

TABLE 61.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*77BER	N	342.6	1	nosp	not specified		C_{avg}	DSIO	*79BER
*81VON		317.3–329.0	3S	nosp	not specified		C_{avg}	DSIO	*81VON

*77BER average value in temperature range 324–361 K

TABLE 61.3.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	317.3–329.0	3	3.00#	0.029	1.65–2	0.09	2.86–5	–1

TABLE 61.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	3	0.050	2.85–2	0.15	2.86–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
317.3–329.0	1.33092+1	1.74226	V

TABLE 61.3.4. Recommended values of heat capacities

Temp. (K)	320	330
c ($J K^{-1} g^{-1}$)	1.07	1.08
C ($J K^{-1} mol^{-1}$)	157	158

Name: Trichloroacetic acid
Formula: $C_2HCl_3O_2$

CAS–RN: 76–03–9
Group No.: 61–004
Molar Mass: 163.39

TABLE 61.4.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*95PIC	N	345.15	1.495	3.70	not specified		C_{avg}	BDHO	*90PIC

*95PIC average value in temperature range 334–356 K

Name: Dichloroacetic acid
Formula: $C_2H_2Cl_2O_2$

CAS–RN: 79–43–6
Group No.: 61–005
Molar Mass: 128.94

TABLE 61.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*95PIC	N	307.1	1	3.70	not specified		C_{avg}	BDHO	*90PIC
02LOU2	N	381.9	1	nosp	not specified		C_{avg}	DSIO	*98LOU

*95PIC average value in temperature range 291–323 K
02LOU2 average value in temperature range 295–469 K

TABLE 61.5.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
02LOU2	381.9	1	5.00#	0.000	0.00	0.00	0.00	0

TABLE 61.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	1	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
381.9–381.9		2.26971+1					VI

TABLE 61.5.4. Recommended values of heat capacities

Temp. (K)	381.90
c ($J\,K^{-1}g^{-1}$)	1.46
C ($J\,K^{-1}mol^{-1}$)	189

Name: Acetyl chloride
Formula: C_2H_3ClO

CAS–RN: 75–36–5
Group No.: 61–006
Molar Mass: 78.50

TABLE 61.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	301.3–317.2	3S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.002	5.40–4	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
301.3–317.2		1.14893+1	8.41034–1				V

TABLE 61.6.4. Recommended values of heat capacities

Temp. (K)	300	310	320
c ($J K^{-1} g^{-1}$)	1.48	1.49	1.50
C ($J K^{-1} mol^{-1}$)	117	117	118

Name: Chloroacetic acid
Formula: $C_2H_3ClO_2$

CAS-RN: 79-11-8
Group No.: 61-007
Molar Mass: 94.50

TABLE 61.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*95PIC	N	342.1	1	3.70	not specified	C_{avg}	BDHO	*90PIC
50URA/SID		335.2–337.7	3	1.00	not specified	C_p	BSIO	50URA/SID

*95PIC average value in temperature range 335–349 K

TABLE 61.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
50URA/SID	335.1–337.7	3	1.00	0.033	9.23–3	0.03	9.17–3	3

TABLE 61.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	3	0.000	0.00	0.00	9.17–3	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
335.1–337.7		9.32756+4	–5.55467+4	8.27200+3			V

TABLE 61.7.4. Recommended values of heat capacities

Temp. (K)	340
c_p ($J K^{-1} g^{-1}$)	3.61
C_p ($J K^{-1} mol^{-1}$)	342

Name: 2,2,2–Trifluoroethanol
Formula: $C_2H_3F_3O$

CAS–RN: 75–89–8
Group No.: 61–008
Molar Mass: 100.04

TABLE 61.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89JAD/FRA	315.0–355.0	5	nosp	99.	anal	C_p	BDCT	86MER/BEN
92MIY/TAM	298.1	1	nosp	99.95	chrom	C_p	FSIO	85OGA

TABLE 61.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
92MIY/TAM	298.1	1	0.30#	0.000	0.00	0.00	0.00	0

TABLE 61.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.13819+1	III

TABLE 61.8.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	1.777
C_p (J K^{-1}mol^{-1})	177.8

Name: 1,1,1,3,3,3–Hexafluoro–2–propanone
Formula: C_3F_6O

CAS–RN: 684–16–2
Group No.: 61–009
Molar Mass: 166.02

TABLE 61.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67PLA/PAC	151.7–244.1	35	nosp	99.991	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 61.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	35	35	0.790	5.06–2	0.24	2.11–4	–5
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
151.7–244.1		2.12324+1	5.66903	–5.71624	1.43066		III

TABLE 61.9.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J K^{-1}g^{-1})	1.087	1.078	1.071	1.065	1.061	1.059	1.061
C_{sat} (J K^{-1}mol^{-1})	180.4	179.0	177.8	176.8	176.1	175.9	176.1
Temp. (K)	220	230	240				
c_{sat} (J K^{-1}g^{-1})	1.065	1.074	1.086				
C_{sat} (J K^{-1}mol^{-1})	176.9	178.3	180.3				

Name: Methyl trichloroacetate
Formula: $C_3H_3Cl_3O_2$

CAS–RN: 598–99–2
Group No.: 61–010
Molar Mass: 177.41

TABLE 61.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	317.6–346.3	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.018	2.23–2	0.09	2.57–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
317.6–346.3		1.53517+1	2.95784				VI

TABLE 61.10.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p (J K^{-1}g^{-1})	1.16	1.18	1.19	1.20
C_p (J K^{-1}mol^{-1})	206	209	211	214

Name: Methyl dichloroacetate
Formula: $C_3H_4Cl_2O_2$

CAS–RN: 116–54–1
Group No.: 61–011
Molar Mass: 142.97

TABLE 61.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	317.6–346.5	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.031	3.62–2	0.15	7.38–5	0

Temp. range K	A_1	A_2	Level of uncertainty
317.6–346.5	1.57185+1	2.33815	VI

TABLE 61.11.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.35	1.36	1.38	1.39
C_p ($J\,K^{-1}mol^{-1}$)	193	195	197	199

Name: Propanoyl chloride
Formula: C_3H_5ClO

CAS–RN: 79–03–8
Group No.: 61–012
Molar Mass: 92.52

TABLE 61.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	312.3–328.5	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.003	1.47–3	0.01	9.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
312.3–328.5		1.83335+1	–2.54307–1				VI

TABLE 61.12.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c ($J K^{-1} g^{-1}$)	1.58	1.57	1.57
C ($J K^{-1} mol^{-1}$)	146	146	145

Name: Methyl chloroacetate
Formula: $C_3H_5ClO_2$

CAS–RN: 96–34–4
Group No.: 61–013
Molar Mass: 108.52

TABLE 61.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*87SCH	309.3–333.9	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.041	4.41–2	0.21	1.18–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
309.3–333.9		1.51805+1	1.96608				VI

TABLE 61.13.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.63	1.65	1.66
C_p ($J\,K^{-1}mol^{-1}$)	177	179	180

Name: (*E*)–3–Chloro–2–butenoic acid
Formula: $C_4H_5ClO_2$

CAS–RN: 6214–28–4
Group No.: 61–014
Molar Mass: 120.54

TABLE 61.14.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
28SKA/SAX	366.75	1.729	nosp	not specified		C_p	DSIO	26AND/LYN

Name: (*Z*)–3–Chloro–2–butenoic acid
Formula: $C_4H_5ClO_2$

CAS–RN: 6213–90–7
Group No.: 61–015
Molar Mass: 120.54

TABLE 61.15.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
28SKA/SAX	333.65	1.652	nosp	not specified		C_p	DSIO	26AND/LYN

Name: 2,2,3–Trichlorobutanal
Formula: $C_4H_5Cl_3O$

CAS–RN: 76–36–8
Group No.: 61–016
Molar Mass: 175.44

TABLE 61.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	323.6–376.7	5S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.138	1.14–1	0.41	5.64–4	1
Temp. range K		A_1	A_2				Level of uncertainty
323.6–376.7		2.60563+1	4.08090–1				VI

TABLE 61.16.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J K^{-1} g^{-1}$)	1.30	1.30	1.30	1.30	1.30	1.31	1.31
C ($J K^{-1} mol^{-1}$)	228	228	228	229	229	229	230

Name: Ethyl trichloroacetate
Formula: $C_4H_5Cl_3O_2$

CAS–RN: 515–84–4
Group No.: 61–017
Molar Mass: 191.44

TABLE 61.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	315.8–375.8	5S	nosp	not specified	C_{avg}	DSIO	*81VON
*87SCH	318.6–347.6	6S	nosp	not specified	C_p	DSIO	*86SCH

TABLE 61.17.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	315.8–375.8	5	5.00#	0.292	4.09–1	1.46	–3.50–1	–5
*87SCH	318.6–347.6	6	5.00#	0.272	4.00–1	1.36	3.12–1	3

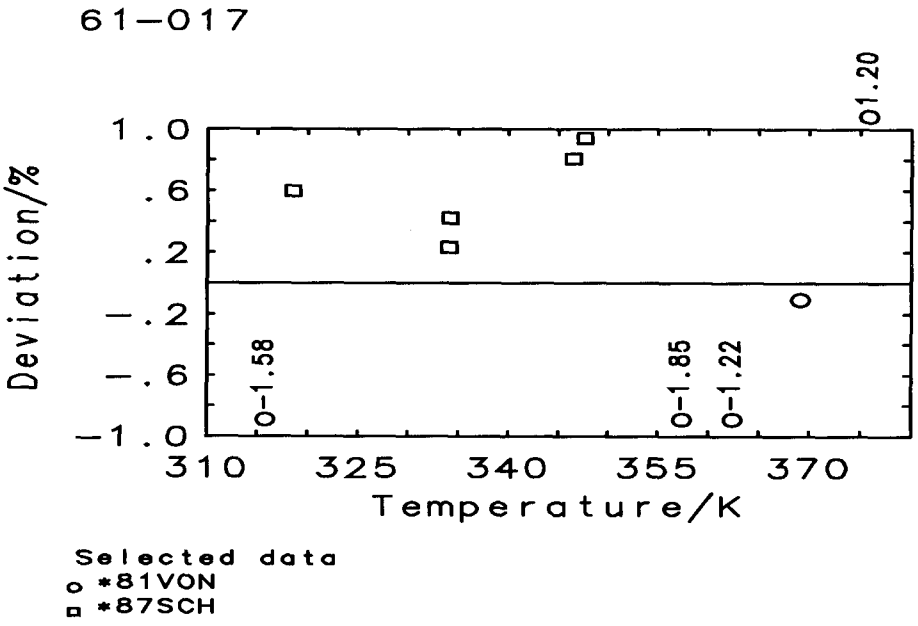
TABLE 61.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.311	4.47–1	1.55	1.14–2	–2
Temp. range K		A_1	A_2				Level of uncertainty
315.8–375.8		2.47051+1	1.19519				V

TABLE 61.17.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1} g^{-1}$)	1.24	1.24	1.25	1.25	1.26	1.27	1.27
C_p ($J K^{-1} mol^{-1}$)	237	238	239	240	241	242	243

0



Name: Ethyl dichloroacetate
Formula: $C_4H_6Cl_2O_2$

CAS–RN: 535–15–9
Group No.: 61–018
Molar Mass: 157.00

TABLE 61.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*81VON	315.9–369.1	5S	nosp	not specified	C_{avg}	DSIO	*81VON
*87SCH	317.5–346.6	6S	nosp	not specified	C_p	DSIO	*86SCH

TABLE 61.18.2. Correlated heat capacities

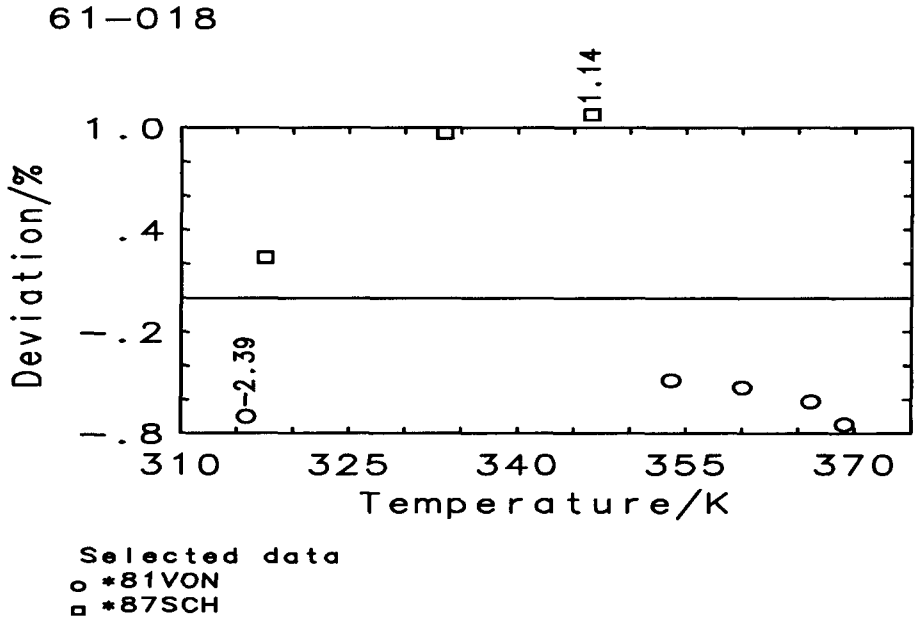
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*81VON	315.9–369.1	5	5.00#	0.240	3.15–1	1.20	–2.55–1	–5
*87SCH	317.5–346.6	6	5.00#	0.187	2.57–1	0.94	2.24–1	6

TABLE 61.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.235	3.15–1	1.18	6.05–3	1
Temp. range K		A_1	A_2				Level of uncertainty
315.9–369.1		2.01457+1	2.05286				V

TABLE 61.18.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.41	1.43	1.44	1.45	1.46	1.47
C_p (J K^{-1}mol^{-1})	222	224	226	227	229	231



Name: Butanoyl chloride
Formula: C_4H_7ClO

CAS–RN: 141–75–3
Group No.: 61–019
Molar Mass: 106.55

TABLE 61.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	317.0–342.5	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.001	1.21–3	0.01	4.77–7	0
Temp. range K		A_1	A_2				Level of uncertainty
317.0–342.5		1.39947+1	2.20863				VI

TABLE 61.19.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J K^{-1} g^{-1}$)	1.64	1.66	1.68
C ($J K^{-1} mol^{-1}$)	175	177	179

Name: 2-Methylpropanoyl chloride
Formula: C_4H_7ClO

CAS-RN: 79-30-1
Group No.: 61-020
Molar Mass: 106.55

TABLE 61.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	319.2–328.7	3S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	3	3	0.002	1.60–3	0.01	6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
319.2–328.7		–4.30167	7.65418				VI

TABLE 61.20.4. Recommended values of heat capacities

Temp. (K)	320	330
c ($J K^{-1} g^{-1}$)	1.58	1.64
C ($J K^{-1} mol^{-1}$)	168	174

Name: Ethyl chloroacetate
Formula: $C_4H_7ClO_2$

CAS–RN: 105–39–5
Group No.: 61–021
Molar Mass: 122.55

TABLE 61.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	309.3–347.0	8S	nosp	not specified	C_p	DSIO	*86SCH

TABLE 61.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.022	2.80–2	0.11	4.15–5	0
Temp. range K		A_1	A_2				Level of uncertainty
309.3–347.0		1.61559+1	2.78454				VI

TABLE 61.21.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.68	1.70	1.72	1.74	1.76
C_p ($J\,K^{-1}mol^{-1}$)	206	208	211	213	215

Name: 1,1'–Oxybis(2–chloroethane)
Formula: $C_4H_8Cl_2O$

CAS–RN: 111–44–4
Group No.: 61–022
Molar Mass: 143.01

TABLE 61.22.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
48TSC1	N	295.1	1	nosp	not specified	C_p	BSIO	48TSC1
49TSC/WET	N	298.1	1	nosp	not specified	C_p	BSIO	49TSC/RIC1
87KAL/KOH		293.1–313.1	2	nosp	99.41 chrom	C_p	FSIT	71PIC/LED

TABLE 61.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
87KAL/KOH	293.1–313.1	2	0.50#	0.000	0.00	0.00	0.00	0
				Rejected data				
48TSC1	(1.15, 4.40, 1.15, 1)			49TSC/WET	(2.73, 9.81, 2.73, 1)			

TABLE 61.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	4	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
293.1–313.1		1.77306+1	2.47760				IV

TABLE 61.22.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.449	1.460	1.463	1.477
C_p ($J\,K^{-1}mol^{-1}$)	207.2	208.8	209.2	211.3

Name: Methyl heptafluorobutanoate
Formula: $C_5H_3F_7O_2$

CAS–RN: 356–24–1
Group No.: 61–023
Molar Mass: 228.07

TABLE 61.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
64VAS1	246.3–305.3	10	nosp	99.9	chrom	C_{sat}	BDAO	64VAS2

TABLE 61.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	10	10	0.677	1.23–1	0.47	4.61–4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
246.4–305.3		1.66156+2	−1.27669+2	2.79734+1			IV

TABLE 61.23.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} ($J\,K^{-1}g^{-1}$)	0.795	0.850	0.925	0.953	1.021	1.136	1.246
C_{sat} ($J\,K^{-1}mol^{-1}$)	181.4	193.9	211.0	217.3	232.8	259.2	284.1
Temp. (K)	300	310					
c_{sat} ($J\,K^{-1}g^{-1}$)	1.273	1.429					
C_{sat} ($J\,K^{-1}mol^{-1}$)	290.2	326.0					

Name: 2–Propenyl trichloroacetate
Formula: $C_5H_5Cl_3O_2$

CAS–RN: 6304–34–3
Group No.: 61–024
Molar Mass: 203.45

TABLE 61.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	316.5–347.0	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.033	5.15–2	0.17	1.08–4	–2
Temp. range K		A_1	A_2				Level of uncertainty
316.5–347.0		1.86447+1	3.73876				VI

TABLE 61.24.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.25	1.27	1.28	1.30
C_p ($J\,K^{-1}mol^{-1}$)	254	258	261	264

Name: 2–Propenyl dichloroacetate
Formula: $C_5H_6Cl_2O_2$

CAS–RN: 30895–77–3
Group No.: 61–025
Molar Mass: 169.01

TABLE 61.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	317.1–347.8	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.027	3.94–2	0.13	6.61–5	0
Temp. range K		A_1	A_2				Level of uncertainty
317.1–347.8		1.82459+1	3.38604				VI

TABLE 61.25.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.43	1.45	1.46	1.48
C_p ($J K^{-1} mol^{-1}$)	242	245	247	250

Name: 2–Propenyl chloroacetate
Formula: $C_5H_7ClO_2$

CAS–RN: 2916–14–5
Group No.: 61–026
Molar Mass: 134.56

TABLE 61.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	317.6–347.8	10S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.031	4.28–2	0.15	1.05–4	–3
Temp. range K		A_1	A_2				Level of uncertainty
317.6–347.8		1.89870+1	2.66311				VI

TABLE 61.26.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.70	1.72	1.73	1.75
C_p ($J K^{-1} mol^{-1}$)	229	231	233	235

Name: Propyl trichloroacetate
Formula: $C_5H_7Cl_3O_2$

CAS–RN: 13313–91–2
Group No.: 61–027
Molar Mass: 205.47

TABLE 61.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	318.2–347.5	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.016	2.57–2	0.08	2.67–5	1
Temp. range K		A_1	A_2				Level of uncertainty
318.2–347.5		1.94929+1	3.83416				VI

TABLE 61.27.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.29	1.30	1.32	1.33
C_p ($J K^{-1} mol^{-1}$)	264	267	270	274

Name: 3,3–Bis(chloromethyl)oxetane
Formula: $C_5H_8Cl_2O$

CAS–RN: 78–71–7
Group No.: 61–028
Molar Mass: 155.02

TABLE 61.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62DAI/EVA	300.0–310.0	2	nosp	not specified		C_p	BSAO	45SCO/MEY

TABLE 61.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
300.0–310.0		1.28837+1	4.47476				IV

TABLE 61.28.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p ($J K^{-1} g^{-1}$)	1.411	1.435
C_p ($J K^{-1} mol^{-1}$)	218.7	222.5

Name: Ethyl 2,3–dichloropropanoate
Formula: $C_5H_8Cl_2O_2$

CAS–RN: 6628–21–3
Group No.: 61–029
Molar Mass: 171.02

TABLE 61.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	N	315.5–380.8	4	nosp	not specified		C_{avg}	DSIO	*81VON

*81VON unspecified isomer; probably 2,3–Dichloropropane (according to n.b.t.)

TABLE 61.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.246	3.85–1	1.23	4.76–3	2
Temp. range K		A_1	A_2				Level of uncertainty
315.5–380.8		2.33634+1	2.18071				VI

TABLE 61.29.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J K^{-1} g^{-1}$)	1.48	1.49	1.50	1.51	1.52	1.53	1.54
C ($J K^{-1} mol^{-1}$)	252	254	256	258	260	261	263

Name: Propyl dichloroacetate
Formula: $C_5H_8Cl_2O_2$

CAS–RN: 37587–81–8
Group No.: 61–030
Molar Mass: 171.02

TABLE 61.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	318.6–348.0	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.018	2.70–2	0.09	3.18–5	0
Temp. range K		A_1	A_2				Level of uncertainty
318.6–348.0		2.01794+1	3.15339				VI

TABLE 61.30.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.47	1.49	1.50	1.52
C_p ($J K^{-1} mol^{-1}$)	252	254	257	260

Name: Pentanoyl chloride
Formula: C_5H_9ClO

CAS–RN: 638–29–9
Group No.: 61–031
Molar Mass: 120.58

TABLE 61.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	313.5–346.9	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.002	2.00–3	0.01	9.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
313.5–346.9		8.23770	5.05374				VI

TABLE 61.31.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350
c ($J K^{-1} g^{-1}$)	1.65	1.68	1.72	1.75	1.79
C ($J K^{-1} mol^{-1}$)	199	203	207	211	216

Name: Ethyl 2–chloropropanoate
Formula: $C_5H_9ClO_2$

CAS–RN: 535–13–7
Group No.: 61–032
Molar Mass: 136.58

TABLE 61.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	321.8–362.3	4S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	4	4	0.026	3.64–2	0.13	4.39–5	0
Temp. range K		A_1	A_2				Level of uncertainty
321.8–362.3		1.94683+1	2.43800				VI

TABLE 61.32.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360
c ($J K^{-1} g^{-1}$)	1.66	1.67	1.69	1.70	1.72
C ($J K^{-1} mol^{-1}$)	227	229	231	233	235

Name: Propyl chloroacetate
Formula: $C_5H_9ClO_2$

CAS-RN: 5396-24-7
Group No.: 61-033
Molar Mass: 136.58

TABLE 61.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*87SCH	318.8–348.2	6S	nosp	not specified		C_p	DSIO	*86SCH

TABLE 61.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.022	3.18-2	0.11	4.80-5	0

Temp. range K	A_1	A_2	Level of uncertainty
318.8–348.2	1.92623+1	3.05611	VI

TABLE 61.33.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.77	1.79	1.81	1.82
C_p ($J K^{-1} mol^{-1}$)	241	244	247	249

Name: Pentafluorophenol
Formula: C_6HF_5O

CAS-RN: 771-61-9
Group No.: 61-034
Molar Mass: 184.07

TABLE 61.34.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
68AND/COU1	315.6–376.9	16	nosp	99.97	melpt	C_p	BSAO	63AND/COU1
69PAU/LAV2	318.0–328.5	4	nosp	98.76	melpt	C_p	BSAO	69PAU/LAV2

TABLE 61.34.2. Correlated heat capacities

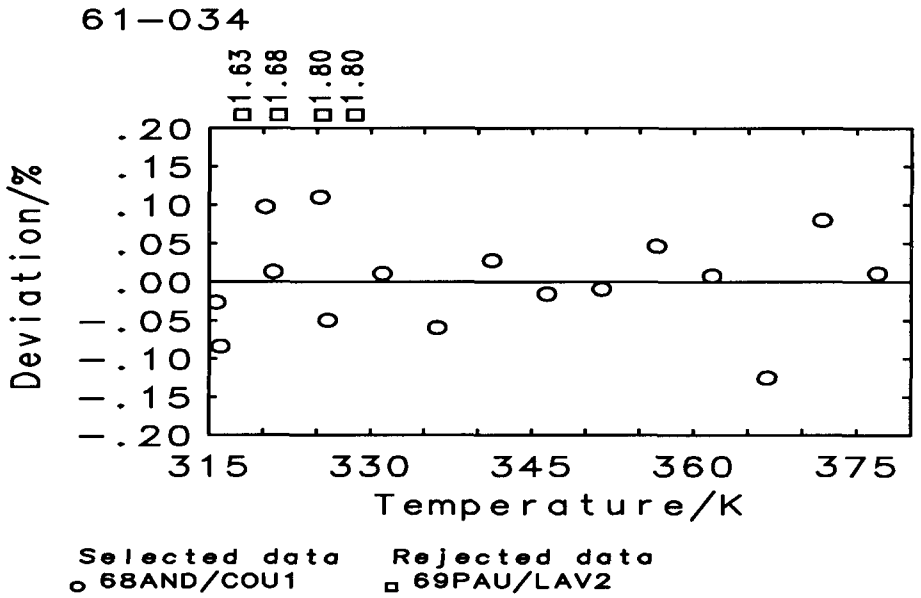
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
68AND/COU1	315.6–376.9	16	0.20#	0.309	2.07-2	0.06	2.81-5	-1
				Rejected data				
69PAU/LAV2	(5.90-1, 1.73, 5.90-1, 4)							

TABLE 61.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	16	0.343	2.29–2	0.07	2.81–5	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
315.6–376.9		5.19043+1	–1.03438+1	1.44241			II

TABLE 61.34.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1}g^{-1}$)	1.517	1.512	1.509	1.507	1.507	1.508	1.510
C_p ($J K^{-1}mol^{-1}$)	279.2	278.4	277.8	277.5	277.4	277.5	277.9



Name: 2,4–Dibromophenol
Formula: $C_6H_4Br_2O$

CAS–RN: 615–58–7
Group No.: 61–035
Molar Mass: 251.91

TABLE 61.35.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*84WER	N	329.65	1.019	nosp	not specified		C_{avg}	DSIO	*79BER

*84WER average value in temperature range 313–346 K; unspecified isomer, probably 2,4–isomer (according to n.m.t.)

Name: 4–Bromophenol
Formula: C_6H_5BrO

CAS–RN: 106–41–2
Group No.: 61–036
Molar Mass: 173.01

TABLE 61.36.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*84WER	N	343.65	1.321	nosp	not specified		C_{avg}	DSIO	*79BER

*84WER average value in temperature range 337–350 K; unspecified isomer, probably 4–isomer (according to n.m.t.)

Name: 2–Chlorophenol
Formula: C_6H_5ClO

CAS–RN: 95–57–8
Group No.: 61–037
Molar Mass: 128.56

TABLE 61.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
16BRA	283.1–323.1	2	nosp	not specified		C_{avg}	DSTO	16BRA
37ELL	298.1–351.1	3S	nosp	not specified		C_p	BSIO	37ELL

TABLE 61.37.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
37ELL	298.1–351.1	3	3.00#	0.050	3.84–2	0.15	1.26–4	1
				Rejected data				
16BRA	(4.16–1, 1.63,–4.16–1, –1)							

TABLE 61.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	3	0.087	6.66–2	0.26	1.26–4	1
Temp. range K		A_1	A_2				Level of uncertainty
298.1–351.1		1.67775+1	2.86465				V

TABLE 61.37.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J\,K^{-1}g^{-1}$)	1.62	1.64	1.64	1.66	1.68	1.70	1.72
C_p ($J\,K^{-1}mol^{-1}$)	209	211	211	213	216	218	220
Temp. (K)	350						
c_p ($J\,K^{-1}g^{-1}$)	1.73						
C_p ($J\,K^{-1}mol^{-1}$)	223						

Name: 4–Fluorophenol
Formula: C_6H_5FO

CAS–RN: 371–41–5
Group No.: 61–038
Molar Mass: 112.10

TABLE 61.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91LIC	N	298.0–354.0	eqn	2.00	99.	anal	C_p	BDCT	89BRE/LIC

91LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 61.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.000	1.48–6	0.00	–3.18–7	0

Temp. range K	A_1	A_2	Level of uncertainty
298.0–354.1	1.82694+1	2.54976	V

TABLE 61.38.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J\,K^{-1}g^{-1}$)	1.92	1.94	1.96	1.98	2.00	2.02
C_p ($J\,K^{-1}mol^{-1}$)	216	218	220	222	224	226

Name: Benzoyl chloride
Formula: C_7H_5ClO

CAS–RN: 98–88–4
Group No.: 61–039
Molar Mass: 140.57

TABLE 61.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*81VON	323.2–387.5	5S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.001	1.27–3	0.01	3.82–7	0

Temp. range K	A_1	A_2	Level of uncertainty
323.2–387.5	1.28397+1	3.21660	VI

TABLE 61.39.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J K^{-1}g^{-1}$)	1.37	1.39	1.41	1.43	1.44	1.46	1.48
C ($J K^{-1}mol^{-1}$)	192	195	198	200	203	206	208

Temp. (K)	390
c ($J K^{-1}g^{-1}$)	1.50
C ($J K^{-1}mol^{-1}$)	211

Name: 2–Chlorobenzoic acid
Formula: $C_7H_5ClO_2$

CAS–RN: 118–91–2
Group No.: 61–040
Molar Mass: 156.57

TABLE 61.40.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	414.0–473.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 61.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
414.0–472.8	2.31548+1	2.81801	VI

TABLE 61.40.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470
c_p ($J K^{-1}g^{-1}$)	1.86	1.87	1.89	1.90	1.92	1.93
C_p ($J K^{-1}mol^{-1}$)	291	293	296	298	300	303

Name: 3–Chlorobenzoic acid
Formula: $C_7H_5ClO_2$

CAS–RN: 535–80–8
Group No.: 61–041
Molar Mass: 156.57

TABLE 61.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	288.0–478.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 61.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
288.0–478.0		3.91250–1	7.54825				VI

TABLE 61.41.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.18	1.22	1.22	1.26	1.30	1.34	1.38
C_p (J K^{-1}mol^{-1})	185	190	192	198	204	210	217
Temp. (K)	350	360	370	380	390	400	410
c_p (J K^{-1}g^{-1})	1.42	1.46	1.50	1.54	1.58	1.62	1.66
C_p (J K^{-1}mol^{-1})	223	229	235	242	248	254	261
Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	1.70	1.74	1.78	1.82	1.86	1.90	1.94
C_p (J K^{-1}mol^{-1})	267	273	279	286	292	298	305

Name: 4–Chlorobenzoic acid
Formula: $C_7H_5ClO_2$

CAS–RN: 74–11–3
Group No.: 61–042
Molar Mass: 156.57

TABLE 61.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	512.8–538.2	2	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN constant value calculated from temperature dependence of enthalpy by the authors

TABLE 61.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
512.8–538.2		4.31307+1					VI

TABLE 61.42.4. Recommended values of heat capacities

Temp. (K)	510	520	530	540
c_p (J K^{-1}g^{-1})	2.29	2.29	2.29	2.29
C_p (J K^{-1}mol^{-1})	359	359	359	359

Name: Bis(2,2,3,3–tetrafluoropropyl) ester carbonic acid
Formula: $C_7H_6F_8O_3$

CAS–RN: 1422–70–4
Group No.: 61–043
Molar Mass: 290.11

TABLE 61.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
80LEB/DOB	256.2–360.2	21	0.30	99.8	chrom	C_p	BSAO	76LEB/LIT

TABLE 61.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	21	21	0.371	5.40–2	0.11	9.68–5	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
256.2–360.2		8.36737+1	–4.32868+1	1.47715+1	–1.47176		III

TABLE 61.43.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.293	1.304	1.308	1.318	1.332	1.345	1.348
C_p ($J K^{-1}mol^{-1}$)	375.1	378.4	379.6	382.2	386.4	390.1	390.9
Temp. (K)	310	320	330	340	350	360	
c_p ($J K^{-1}g^{-1}$)	1.364	1.381	1.399	1.416	1.434	1.451	
C_p ($J K^{-1}mol^{-1}$)	395.7	400.7	405.7	410.8	415.9	420.8	

Name: 2,2,3,3,4,5,5–Heptafluorotetrahydro–4–(nonafluorobutyl)furan
Formula: $C_8F_{16}O$

CAS–RN: 646–85–5
Group No.: 61–044
Molar Mass: 416.06

TABLE 61.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
57YAR/KAY	305.0–368.0	eqn	1.10	not specified		C_p	BSIO	75PED/KAY

TABLE 61.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.000	3.82–6	0.00	9.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
305.0–368.0		2.55438+1	8.81445				V

TABLE 61.44.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J K^{-1}g^{-1}$)	1.06	1.07	1.09	1.11	1.13	1.14	1.16
C_p ($J K^{-1}mol^{-1}$)	440	447	454	462	469	476	484

Name: 1,2–Benzenedicarbonyl dichloride
Formula: $C_8H_4Cl_2O_2$

CAS–RN: 88–95–9
Group No.: 61–045
Molar Mass: 203.02

TABLE 61.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	317.2–384.9	5S	nosp	not specified		C_{avg}	DSIO	*81VON

TABLE 61.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	5	5	0.002	2.67–3	0.01	–3.82–7	–1

Temp. range K	A_1	A_2	Level of uncertainty
317.2–384.9	1.87550+1	3.73118	VI

TABLE 61.45.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c ($J K^{-1}g^{-1}$)	1.26	1.27	1.29	1.30	1.32	1.33	1.35
C ($J K^{-1}mol^{-1}$)	255	258	261	265	268	271	274

Name: 2–Chloro–3–phenyl–2–propenal
Formula: C_9H_7ClO

CAS–RN: 18365–42–9
Group No.: 61–046
Molar Mass: 166.61

TABLE 61.46.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
08BOG/WIN	N	314.15	1.653	nosp	not specified		C_{avg}	DSIO	08BOG/WIN

08BOG/WIN average value in temperature range 305–323 K

62. Compounds of Carbon, Hydrogen, Nitrogen and Oxygen

This family contains 127 compounds of which 28 were measured at one temperature only. In this monograph, two compounds were listed only in the table Experimental Heat Capacities, but no temperature correlation or recommendations were performed because the data are obviously erroneous and come from measurements at RAB (78MAR/CIO1).

The large number of data in this family corresponds to the importance and use of many compounds both in industry and in research. Most of the data were measured at JHUB where parameters of a linear equation were published for 10 nitro compounds (23AND/LYN). The authors did not give any information regarding measurement errors or purity of samples. Hence, the recommended data have been assigned the highest level of uncertainty.

Six compounds were measured at NIPER (formerly BMB) (89STE/CHI3, 90STE/CHI, 92STE/CHI2), two of which at one temperature only. For 1-methyl-2-pyrrolidinone the reported value has been discarded as it was obviously erroneous (a probable misprint). Benzoxazole (92STE/CHI2) was measured over the entire temperature range from the triple point to the close vicinity of the critical temperature using two instruments (adiabatic and DSC calorimeters with reported errors of 0.1 and 1 %, respectively).

Measurements for formamide, acetamide, 2-cyanoacetamide, and the ethyl ester of carbamic acid were carried out over a narrow temperature range at SUU (83DEW/DEK, 83DEW/OFF); the resulting data showed an uncertainty up to 0.5 %. Three diamides were studied at NWUE (53WIL/DOL) and two esters of nitric acid were investigated jointly at UCE and UOE (53GRA/SMI, 54GRA/SMI), the estimated uncertainty varied in all cases from 0.5 to 1 %. Data for 2,2-dinitropropane (78GOD/RAC) were published as a graph only and the numerical values of heat capacity were provided to us through courtesy of the authors from the Institute of Physics, Cracow, Poland.

Several compounds from this family were measured in fSU. Probably the most reliable data were obtained at MSUM for heterocyclic compounds (62KOL/PAU, 63KOL/PAU), and for diisocyanates and *N*,*N*-dimethylacetamide from studies at CIUG (73MOS/NIK, 77LEB/EVS3, 85LEB/BYK). Heat capacities of isopropyl ester of nitric acid were measured at the Institute of Chemical Physics of the Academy of Sciences, Chernogolovka near Moscow (88LUS/RUB); the authors claim a very low experimental error (0.05 %) which we consider not to be real due to the low purity of the sample used.

It is difficult to evaluate the uncertainty of data published in the form of parameters of an equation as in these cases authors do not usually give any details regarding scatter of data and measurement procedures. This is frequently the case for data from fSU laboratories such as: 6 compounds (three isomers of nitrophenol, three isomers of 1-methoxynitrobenzene) investigated at PIK (58LUT/PAN, 59LUT/PAN) and five esters of phenylcarbamic acid studied at the Institute of Highmolecular Compounds, Soviet Academy of Sciences in Kiev (71PRI). A large quantity of both experimental or/and smoothed data was published by two Azerbaidzhanian laboratories (fSU): ANAZ (79DZA/KAR, 83GEI/KAR, 84GEI/KAR) and APIB (81MUS/GAN) which claimed errors below 0.2 and 0.5 %, respectively. However, it is very difficult to judge what is the real reliability of the data because most information is confusing and the data for most of the investigated compounds were reported in literature only once, hence, comparison with independent sources is impossible. Comparison was possible in the case of 4-oxobutanenitrile which was studied in both above laboratories with results differing by 9 %. Such a disagreement indicates the possibility of large systematic errors.

Some industrially important compounds were measured at BSU (88KOZ/KRA, 89KOZ/MAR, 90KOZ/SIM, 91KOZ/MAR, 92KAB/KOZ). The reported uncertainty of 2 % for the data which were presented as parameters of a polynomial equation seems to be reasonable with the exception of the data for ϵ-caprolactam. For this compound, the BSU laboratory published parameters of an equation in two papers (89KOZ/MAR, 92KAB/KOZ); the resulting data differed by 20 % from each other. The values in the former source agreed reasonably with another independent source from MSUM (62KOL/PAU), and therefore, are probably more reliable.

Data for 4,4'-oxybisbenzenamine were measured with reasonable accuracy at LCSP (87LES/LIC). These results have helped us to reveal enormous errors of the C_p data from RAB (78MAR/CIO1), where heat capacities were derived from the measured enthalpy as a function of temperature. The shape of the $C_p = f(T)$ curve and the published values are completely unrealistic. The same also applies to the data for compounds from other families reported in the latter source. We have listed this source only for the completeness of our literature survey but have never included the data in the correlation even if no other data were available.

Dimethylformamide was the most frequently measured substance in this family. However, most data are available at one temperature only (298.15 K) and were obtained as a part of excess heat capacity measurements. For our recommendations, we have selected the low temperature data from CIUG (73MOS/NIK) and the compiled and smoothed data from Du Pont de Nemours & Co, Wellington, USA (70ANO) between room temperature and the normal boiling temperature (432.2 K) where no direct experimental data were accessible. In the latter source, neither the type of heat capacity nor the experimental device were given and we have presented, therefore, only one set of recommended values which are probably C_{sat}. The authors from IKNR (89PET/PES) reported a minimum on the curve $C_p = f(T)$ at 278 K; this phenomenon was not confirmed by other authors, and therefore, the above data have been rejected from the final correlation. However, it is not possible to unequivocally discard a possibility of a minimum on the heat capacity curve of dimethylformamide as a minimum was certainly found at GITA (66LIN/ZIE) for nitroethane where reliable data (claimed uncertainty 0.4 %) are available. The general discussion of extremes of heat capacity data can be found in the reference (93ZAB/BUR).

Nitromethane was frequently measured also. We have selected the reliable low temperature data from UCB (47JON/GIA) and the high quality data from NBSW (69BER/WES) that extend the C_p data 100 K above the normal boiling temperature.

Nitrobenzene is the third most frequently measured compound from this family. We have selected two sets of older data from a Polish laboratory (39MAZ1, 39MAZ3) covering a narrow temperature interval (20 K), the data from PIK (58LUT/PAN) near ambient temperatures, and also the high-temperature measurements from GPI (67RAS/GAN). All three sources have comparable errors ranging from 0.5 to 1 %.

A certain number of compounds in this family belong to a class of substances called liquid crystals. The melting of liquid crystals occurs in several stages that differ by the ordering of the molecules in the liquid state. We have included only data relating to the true liquid (isotropic) state. The temperature dependence of the heat capacity for liquid crystals differs from that of most other organic compounds. The heat capacity first drops sharply to a minimum and then slowly starts rising almost linearly with temperature. A mathematical description of this type of dependence by a polynomial of the second or third degree is difficult. Using cubic spline polynomials was not appropriate due to the narrow temperature range of data for an isotropic liquid. The assigned level of accuracy reflects more the quality of the description of $C_p = f(T)$ curve by a polynomial than the quality of experimental data. Mainly Japanese laboratories, such as OCUO (73SOR/SEK, 74SOR/NAK, 79TSU/SOR, 82TSU/SOR4, 83SOR/TAN, 83YOS/SOR2) or NCLT (74SHI/MAE) were involved in this research in the seventies and eighties and the reliability of data is generally very good. Measurements from MLUH (64ARN2) for 12 liquid crystals were published as discrete experimental data points up to the minimum in the heat capacity and at higher temperatures as parameters of a linear equation, but without any indication of error. In another study for which data were obtained at the Academy of Science the Bellorussian SSR, Minsk (85SHA/ZHU) results for two compounds were published over a very narrow temperature interval.

Name: Formamide
Formula: CH_3NO

CAS–RN: 75–12–7
Group No.: 62–001
Molar Mass: 45.04

TABLE 62.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
65SOM/COO	N	298.1	1	0.20	not specified		C_p	BSAO	56COO/BAL
66EGA/LUF		298.1	1	nosp	not specified		C_p	BSIO	61EGA/LUF
67RAS/GAN		293.1–373.1	5S	0.50	not specified		C_p	BSAO	67RAS/GAN
74DEV/SOM	N	298.1	1	0.50	not specified		C_p	BSIO	70LKB/COM
76BON/CER		298.1	1	nosp	not specified		C_p	BSIO	76BON/CER
76SKO/SUU		298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU
77VOR/PRI		297.4	1	0.80	not specified		C_{sat}	BSAO	77VOR/PRI
78DEV/HEU		298.1	1	1.00	99.8	chrom	C_p	BSIO	70LKB/COM
83DEW/DEK		276.8–293.7	8	nosp	99.57	melpt	C_p	BSAO	79SCH/OFF

65SOM/COO high purity of substance with water content below 0.02 %
74DEV/SOM C_p values for Formamide and *N*,*N*–Dimethylformamide were interchanged

TABLE 62.1.2. Correlated heat capacities

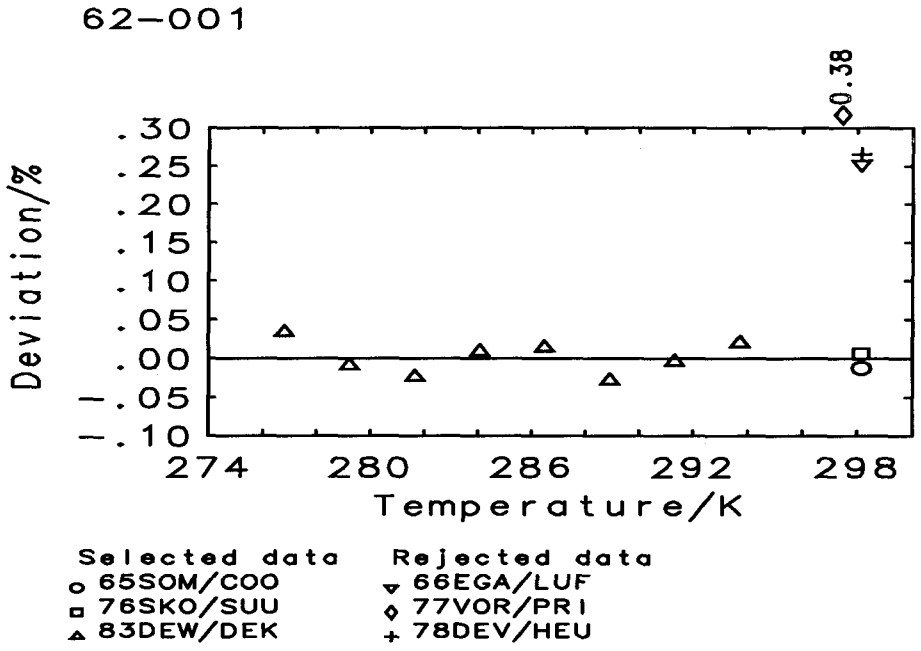
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
65SOM/COO	298.1	1	0.20	0.073	1.89–3	0.01	–1.89–3	–1
76SKO/SUU	298.1	1	0.10	0.040	5.12–4	0.00	5.12–4	0
83DEW/DEK	276.8–293.7	8	0.50#	0.040	2.58–3	0.02	–1.19–4	0
				Rejected data				
66EGA/LUF	(3.25–2, 0.25, 3.25–2, 1)			67RAS/GAN	(2.58–1, 2.04, –2.58–1, –1)			
74DEV/SOM	(5.82–2, 0.45, 5.82–2, 1)			76BON/CER	(7.41–2, 0.58, –7.41–2, –1)			
77VOR/PRI	(4.88–2, 0.38, 4.88–2, 1)			78DEV/HEU	(3.42–2, 0.26, 3.42–2, 1)			

TABLE 62.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	10	0.050	2.68–3	0.02	–2.34–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
276.8–298.1		1.07961+1	7.20102–1				IV

TABLE 62.1.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300
c_p (J K^{-1}g^{-1})	2.365	2.378	2.389	2.392
C_p (J K^{-1}mol^{-1})	106.5	107.1	107.6	107.7



Name: Nitromethane
Formula: CH_3NO_2

CAS–RN: 75–52–5
Group No.: 62–002
Molar Mass: 61.04

TABLE 62.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
07WAL	290.1	1	nosp	not specified		C_{avg}	DSIO	07WAL
47JON/GIA	249.8–297.1	11	nosp	99.7	melpt	C_p	BSIO	37GIA/EGA
50HOU/MAS2	313.1–363.1	6S	0.40	99.8	estim	C_p	BSAO	50SAG/HOU
65ZIE N	316.0–333.9	2	nosp	not specified		C_{avg}	DSIO	58SWI/ZIE1
69BER/WES	308.1–473.1	18S	0.10	99.99	melpt	C_{sat}	BSAO	68WES/WES

65ZIE average values in temperature ranges 294–374 K and 294–338 K

TABLE 62.2.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
47JON/GIA	249.8–297.1	11	0.40#	0.394	2.00–2	0.16	–3.99–3	1
69BER/WES	308.1–473.1	18	0.10	0.140	1.93–3	0.01	1.55–4	1
				Rejected data				
07WAL	(6.94–2, 0.55,–6.94–2, –1)			50HOU/MAS2	(1.33–1, 01.00, 1.31–1, 6)			
65ZIE	(2.79–1, 2.19,–2.74–1, –2)							

TABLE 62.2.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	29	0.293	1.36–2	0.11	–1.42–3	2
C_{sat}	38	29	0.304	1.40–2	0.11	–1.57–3	1

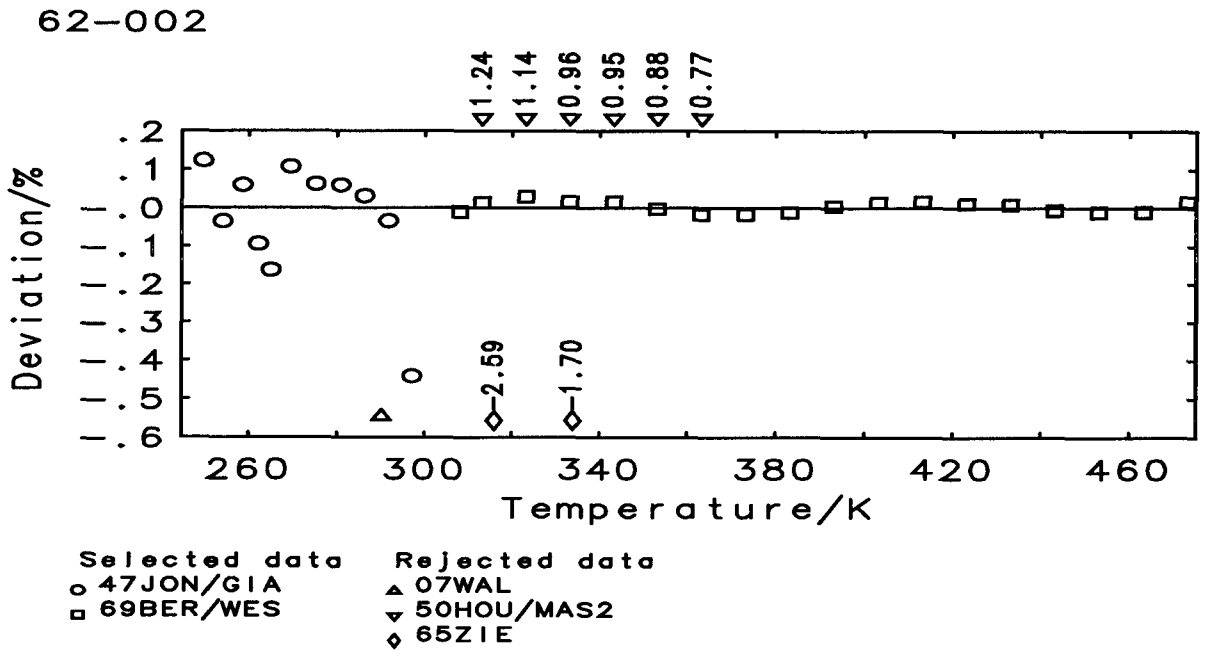
Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
249.8–360.0	2.12369+1	–8.25090	2.40747	–1.98146–1	III
360.0–473.2	–1.43585	1.06430+1	–2.84085	2.87809–1	III
249.8–360.0	2.07973+1	–7.87297	2.30443	–1.89442–1	III
360.0–473.2	2.85957	7.07512	–1.84782	1.95025–1	III

TABLE 62.2.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.711	1.713	1.718	1.720	1.724	1.733	1.742
C_p (J K^{-1}mol^{-1})	104.4	104.6	104.8	105.0	105.3	105.8	106.3
c_{sat} (J K^{-1}g^{-1})	1.710	1.713	1.718	1.720	1.725	1.733	1.742
C_{sat} (J K^{-1}mol^{-1})	104.4	104.6	104.9	105.0	105.3	105.8	106.3
Temp. (K)	**300**	**310**	**320**	**330**	**340**	**350**	**360**
c_p (J K^{-1}g^{-1})	1.744	1.756	1.770	1.785	1.802	1.819	1.837
C_p (J K^{-1}mol^{-1})	106.4	107.2	108.0	109.0	110.0	111.0	112.2
c_{sat} (J K^{-1}g^{-1})	1.744	1.756	1.770	1.785	1.801	1.818	1.836
C_{sat} (J K^{-1}mol^{-1})	106.5	107.2	108.0	109.0	109.9	111.0	112.1
Temp. (K)	**370**	**380**	**390**	**400**	**410**	**420**	**430**
c_p (J K^{-1}g^{-1})	1.857	1.877	1.898	1.921	1.945	1.972	2.000
C_p (J K^{-1}mol^{-1})	113.3	114.6	115.9	117.3	118.7	120.4	122.1
c_{sat} (J K^{-1}g^{-1})	1.855	1.875	1.896	1.917	1.941	1.965	1.992
C_{sat} (J K^{-1}mol^{-1})	113.2	114.4	115.7	117.0	118.5	120.0	121.6
Temp. (K)	**440**	**450**	**460**	**470**			
c_p (J K^{-1}g^{-1})	2.031	2.065	2.101	2.140			
C_p (J K^{-1}mol^{-1})	124.0	126.0	128.2	130.6			
c_{sat} (J K^{-1}g^{-1})	2.020	2.050	2.082	2.117			
C_{sat} (J K^{-1}mol^{-1})	123.3	125.1	127.1	129.2			

TABLE 62.2.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_t %	s_b/R	+/–
C_p	38	29	1.734	7.23–2	0.57	2.80–2	7
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
249.8–473.1	588.00	–1.38108	4.78386–1	1.03417+1	9.96779–1		IV



Name: Methyl ester nitric acid
Formula: CH_3NO_3

CAS-RN: 598-58-3
Group No.: 62-003
Molar Mass: 77.04

TABLE 62.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
53GRA/SMI	193.7–295.5	10	nosp	not specified	C_p	BSIO	51PAR/SIM

TABLE 62.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.634	8.84-2	0.51	6.41-4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
193.7–295.5		-7.99832	1.83078+1	-3.12434			V

TABLE 62.3.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	1.74	1.80	1.85	1.90	1.94	1.97	1.99
C_p ($J K^{-1}mol^{-1}$)	134	139	143	146	149	152	154
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J K^{-1}g^{-1}$)	2.01	2.02	2.03	2.03	2.03	2.03	
C_p ($J K^{-1}mol^{-1}$)	155	155	156	156	156	156	

Name: Urea
Formula: CH_4N_2O

CAS-RN: 57-13-6
Group No.: 62-004
Molar Mass: 60.06

TABLE 62.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
80VOG/SCH	N	413.0–425.0	eqn	nosp	not specified	C_p	BDHT	69PER/COM
80VOG/SCH	N	413.0–425.0	eqn	nosp	not specified	C_p	BDHT	69PER/COM
88GAM/BRO		411.1	1	1.00	99.5 anal	C_p	BDCT	86MER/BEN

80VOG/SCH dried sample contained a high amount of biuret
80VOG/SCH undried sample contained 0.065 mol.% of biuret

TABLE 62.4.2. Correlated heat capacities

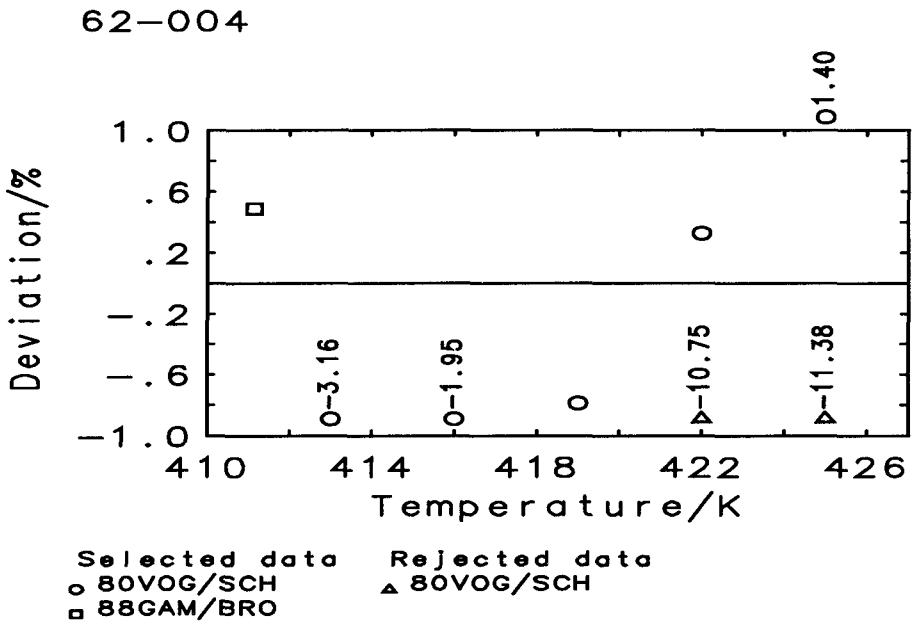
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
80VOG/SCH	413.0–425.0	5	3.00#	0.605	3.19–1	1.82	–1.42–1	–1
88GAM/BRO	411.1	1	1.00	0.486	8.66–2	0.49	8.66–2	1
				Rejected data				
80VOG/SCH	(1.68, 10.16, –1.67, –5)							

TABLE 62.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	6	0.719	3.60–1	2.05	–1.04–1	0
Temp. range K		A_1	A_2				Level of uncertainty
411.1–425.0		–5.65733	5.68721				V

TABLE 62.4.4. Recommended values of heat capacities

Temp. (K)	410	420	430
c_p (J K^{-1}g^{-1})	2.45	2.52	2.60
C_p (J K^{-1}mol^{-1})	147	152	156



Name: Acetamide
Formula: C_2H_5NO

CAS–RN: 60–35–5
Group No.: 62–005
Molar Mass: 59.07

TABLE 62.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DEW/DEK		355.9–363.1	4	nosp	99.99	melpt	C_p	BSAO	79SCH/OFF
85VOG/SCH	N	360.0–390.0	eqn	nosp	not specified		C_p	BDHT	69PER/COM
86EMO/NAU	N	370.0–400.0	4S	nosp	not specified		C_p	BDHT	87PER/COM

85VOG/SCH suspect equation
86EMO/NAU water content 0.07 mol.%

TABLE 62.5.2. Correlated heat capacities

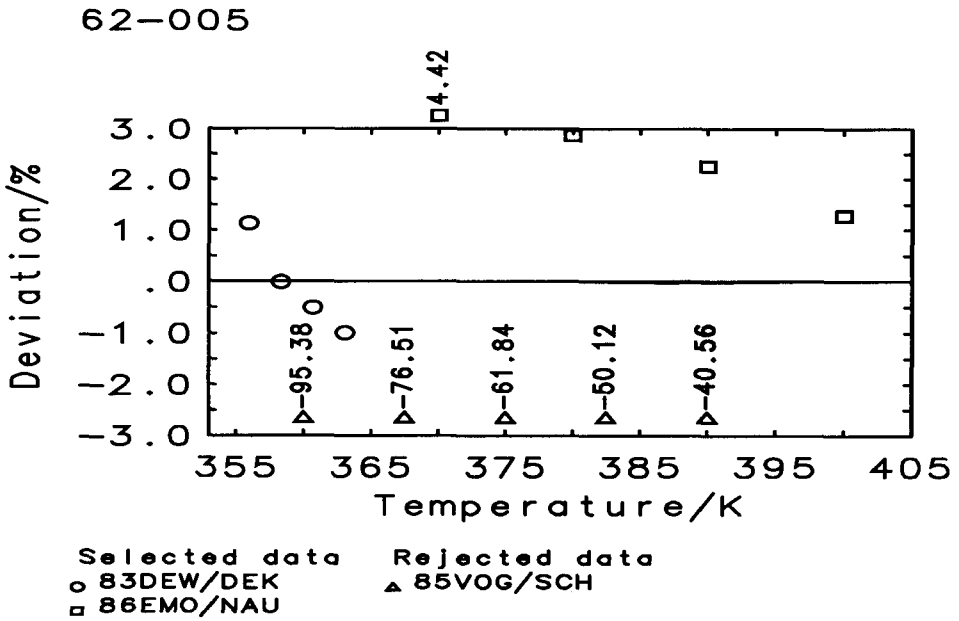
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83DEW/DEK	355.9–363.1	4	0.40#	1.989	1.48–1	0.80	–1.83–2	–2
86EMO/NAU	370.0–400.0	4	2.00#	1.466	5.95–1	2.93	5.52–1	4
				Rejected data				
85VOG/SCH	(7.55, 67.73, –7.47, –5)							

TABLE 62.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	8	2.018	5.01–1	2.48	2.67–1	2
Temp. range K		A_1	A_2				Level of uncertainty
355.9–400.0		–1.03027	5.47042				V

TABLE 62.5.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400
c_p ($J K^{-1} g^{-1}$)	2.63	2.70	2.78	2.86	2.94
C_p ($J K^{-1} mol^{-1}$)	155	160	164	169	173



Name: *N*–Methylformamide
Formula: C_2H_5NO

CAS–RN: 123–39–7
Group No.: 62–006
Molar Mass: 59.07

TABLE 62.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
74DEV/SOM	298.1	1	0.50	not specified	C_p	BSIO	70LKB/COM
76BON/CER	298.1	1	nosp	not specified	C_p	BSIO	76BON/CER
76SKO/SUU	298.1	1	0.10	not specified	C_p	DDCT	71KON/SUU
79DEV/SOM	298.1	1	1.00	99.8 chrom	C_p	BSIO	70LKB/COM
89KUL/KRE	308.0	1	nosp	not specified	C_p	BSAO	83KUK/KOR

TABLE 62.6.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
76BON/CER	298.1	1	1.00#	1.472	2.16–1	1.47	–2.16–1	–1
76SKO/SUU	298.1	1	0.10	0.038	5.71–4	0.00	5.71–4	0
79DEV/SOM	298.1	1	1.00	1.122	1.69–1	1.12	1.69–1	1
89KUL/KRE	308.0	1	0.50#	0.000	0.00	0.00	0.00	0
				Rejected data				
74DEV/SOM	(2.77–1, 1.83, 2.77–1, 1)							

TABLE 62.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	5	4	1.309	1.94–1	1.31	–1.16–2	0
Temp. range K		A_1	A_2				Level of uncertainty
298.1–308.0		4.56915	3.46132				IV

TABLE 62.6.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310
c_p (J K^{-1}g^{-1})	2.056	2.096	2.105	2.154
C_p (J K^{-1}mol^{-1})	121.4	123.8	124.3	127.2

Name: Nitroethane
Formula: $C_2H_5NO_2$

CAS–RN: 79–24–3
Group No.: 62–007
Molar Mass: 75.07

TABLE 62.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
66LIN/ZIE	N	188.6–300.3	38	0.40	99.92	melpt	C_{sat}	BSAO	63ZIE/MUL

66LIN/ZIE purity 99.2 % (chromatographic analysis), principal impurity 2–Nitropropane

TABLE 62.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	38	38	0.179	1.13–2	0.07	1.59–5	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
188.6–300.3		3.06331+1	–1.63197+1	5.64510	–6.04653–1		III

TABLE 62.7.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_{sat} (J K^{-1}g^{-1})	1.756	1.743	1.734	1.729	1.728	1.730	1.735
C_{sat} (J K^{-1}mol^{-1})	131.8	130.8	130.2	129.8	129.7	129.9	130.3
Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.743	1.752	1.756	1.764	1.776	1.787	1.789
C_{sat} (J K^{-1}mol^{-1})	130.8	131.5	131.8	132.4	133.3	134.1	134.3

TABLE 62.7.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	38	23	0.111	7.03–3	0.04	3.44–6	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
229.4–300.3	592.00	4.93089+1	1.86881+1	–3.34811	3.25257+1		III

Name: Ethyl nitrate
Formula: $C_2H_5NO_3$

CAS–RN: 625–58–1
Group No.: 62–008
Molar Mass: 91.07

TABLE 62.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
54GRA/SMI	182.0–293.0	15	nosp	not specified	C_p	BSIO	51PAR/SIM

TABLE 62.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	1.074	2.14–1	1.07	3.99–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
182.0–293.0		1.84251+1	6.71384–1				V

TABLE 62.8.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.79	1.80	1.80	1.81	1.82	1.82	1.83
C_p (J K^{-1}mol^{-1})	163	164	164	165	165	166	167
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.84	1.84	1.85	1.85	1.85	1.86	1.86
C_p (J K^{-1}mol^{-1})	167	168	168	168	169	169	170

Name: Nitrate ethylamine
Formula: $C_2H_8N_2O_3$

CAS–RN: 22113–86–6
Group No.: 62–009
Molar Mass: 108.10

TABLE 62.9.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
85ALL/EVA	N	298.15	1.902	nosp	not specified	C_p	FSIT	71PIC/LED

85ALL/EVA extrapolated values from measurements with aqueous solution (highest concentration: 99.916 mass.%)

Name: Isoxazole
Formula: C_3H_3NO

CAS–RN: 288–14–2
Group No.: 62–010
Molar Mass: 69.06

TABLE 62.10.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78MCC/HAM	298.15	1.343	nosp	not specified		C_p	BDHT	73PER/COM

Name: Oxazole
Formula: C_3H_3NO

CAS–RN: 288–42–6
Group No.: 62–011
Molar Mass: 69.06

TABLE 62.11.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78MCC/HAM	298.15	1.397	nosp	not specified		C_p	BDHT	73PER/COM

Name: 2–Cyanoacetamide
Formula: $C_3H_4N_2O$

CAS–RN: 107–91–5
Group No.: 62–012
Molar Mass: 84.08

TABLE 62.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83DEW/OFF	405.0–420.0	4S	nosp	not specified		C_p	BDHT	69PER/COM

TABLE 62.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.045	2.14–2	0.09	1.91–5	0
Temp. range K		A_1	A_2				Level of uncertainty
405.0–420.0		1.58742+1	1.85404				V

TABLE 62.12.4. Recommended values of heat capacities

Temp. (K)	400	410	420
c_p ($J\,K^{-1}g^{-1}$)	2.30	2.32	2.34
C_p ($J\,K^{-1}mol^{-1}$)	194	195	197

Name: 2–Propenamide
Formula: C_3H_5NO

CAS–RN: 79–06–1
Group No.: 62–013
Molar Mass: 71.08

TABLE 62.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI3	365.0–415.0	6	1.00	99.99	chrom	C_{sat}	BDHT	89KNI/ARC

TABLE 62.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	6	6	0.143	3.31–2	0.14	6.74–5	–2

Temp. range K	A_1	A_2	Level of uncertainty
365.0–415.0	1.32700+1	2.54301	IV

TABLE 62.13.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390	400	410	420
c_{sat} (J K^{-1}g^{-1})	2.623	2.653	2.683	2.712	2.742	2.772	2.802
C_{sat} (J K^{-1}mol^{-1})	186.5	188.6	190.7	192.8	194.9	197.0	199.1

Name: Methyl ester nitroacetic acid
Formula: $C_3H_5NO_4$

CAS–RN: 2483–57–0
Group No.: 62–014
Molar Mass: 119.08

TABLE 62.14.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEB/RYA	N	320.50	1.728	1.00	not specified		C_{avg}	DSIO	76LEB/RYA

81LEB/RYA average value in temperature range 298–343 K

Name: 2,2–Dinitropropane
Formula: $C_3H_6N_2O_4$

CAS–RN: 595–49–3
Group No.: 62–015
Molar Mass: 134.09

TABLE 62.15.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78GOD/RAC	N	326.4–344.5	13	nosp	99.8	estim	C_p	BSAO	71MAY/WAL

78GOD/RAC only a graph given in the paper; experimental values provided by the authors

TABLE 62.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.545	2.14–1	0.82	2.98–3	4
Temp. range K		A_1	A_2				Level of uncertainty
326.4–344.5		2.16706+1	1.39554				V

TABLE 62.15.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p ($J K^{-1} g^{-1}$)	1.63	1.64
C_p ($J K^{-1} mol^{-1}$)	218	220

Name: *N*,*N*–Dimethylformamide
Formula: C_3H_7NO

CAS–RN: 68–12–2
Group No.: 62–016
Molar Mass: 73.09

TABLE 62.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type Reference
61GEL		273.0–323.0	5S	nosp	not specified	C_p	not specified
70ANO		293.2–423.2	8S	nosp	not specified	C_{sat}	not specified
73MOS/NIK		212.6–298.1	4S	nosp	99.5 melpt	C_p	BSAO 66NIK/LEB
74DEV/SOM	N	298.1	1	0.50	not specified	C_p	BSIO 70LKB/COM
76BON/CER		298.1	1	nosp	not specified	C_p	BSIO 76BON/CER
77BON/BED	N	298.1	1	0.10	not specified	C_p	BSIO 76BON/CER
77DEV/PER2		298.1	1	0.30	not specified	C_p	FSIT 71PIC/LED
77DEV/PER3		298.1	1	0.50	not specified	C_p	FSIT 71PIC/LED
77VYU		298.0	1	nosp	not specified	C_p	not specified
78MAR/CIO1	N	298.1–429.1	2	nosp	not specified	C_p	DSIO 71MAR/CIO
79DEV/SOM		298.1	1	1.00	99.8 chrom	C_p	BSIO 70LKB/COM
82VOR/YAK		298.1	1	nosp	not specified	C_p	BSAO 77VOR/PRI
84ZEG/SOM2		298.1	1	0.30	99.5 chrom	C_p	FSIT 71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified	C_p	BSAO 83KUK/KOR
87PIE		298.1	1	nosp	99.5 chrom	C_p	FSIT 71PIC/LED
89KUL/KRE		308.0	1	nosp	not specified	C_p	BSAO 83KUK/KOR
89PET/PES		258.1–318.1	4	nosp	not specified	C_p	BSAO 83KUK/KOR
91GRO/ROU		298.1	1	nosp	99.5 anal	C_p	FSIT 71PIC/LED

74DEV/SOM C_p values for *N*,*N*–Dimethylformamide and Formamide were interchanged
77BON/BED infrared spectrum indicated that sample was water–free
78MAR/CIO1 constant value calculated from temperature dependence of enthalpy by the authors

TABLE 62.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70ANO	293.2–423.2	8	1.50#	0.819	2.29–1	1.23	1.83–1	6
73MOS/NIK	212.6–298.1	4	0.50#	0.823	7.12–2	0.41	1.20–2	0
77DEV/PER2	298.1	1	0.30	0.408	2.18–2	0.12	–2.18–2	–1
77DEV/PER3	298.1	1	0.50	0.025	2.27–3	0.01	2.27–3	1
84ZEG/SOM2	298.1	1	0.30	0.402	2.15–2	0.12	2.15–2	1
86KOR/KUK	278.0–298.0	2	0.20	2.193	7.76–2	0.44	–1.58–2	0
87PIE	298.1	1	0.50#	0.242	2.15–2	0.12	2.15–2	1
89KUL/KRE	308.0	1	0.50#	0.219	1.96–2	0.11	–1.96–2	–1
				Rejected data				
61GEL	(1.43, 7.37, 1.28, 5)			74DEV/SOM	(4.59–1, 2.51, 4.59–1, 1)			
76BON/CER	(2.62–1, 1.49,–2.62–1, –1)			77BON/BED	(3.31–1, 1.89, –3.31–1, –1)			
77VYU	(4.31–1, 2.36, 4.31–1, 1)			78MAR/CIO1	(3.33, 22.97, –3.33, –1)			
79DEV/SOM	(3.15–1, 1.74, 3.15–1, 1)			82VOR/YAK	(2.79–1, 1.54, 2.79–1, 1)			
89PET/PES	(4.60–1, 2.54, 3.77–1, 4)			91GRO/ROU	(2.56–1, 1.46, –2.56–1, –1)			

TABLE 62.16.3. Parameters of regression polynomial

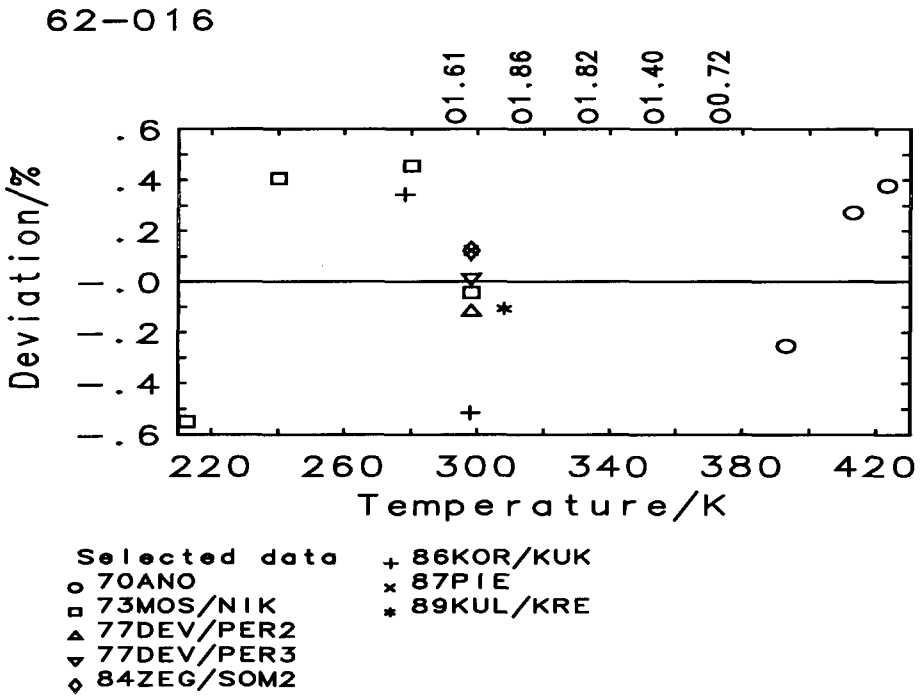
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	37	19	1.064	1.68–1	0.91	7.80–2	7
Temp. range K		A_1	A_2	A_3			Level of uncertainty
212.6–423.2		2.05390+1	–3.28542	7.96284–1			V

TABLE 62.16.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c ($J K^{-1} g^{-1}$)	1.95	1.96	1.96	1.97	1.98	1.99	1.99
C ($J K^{-1} mol^{-1}$)	143	143	143	144	145	145	146
Temp. (K)	280	290	298.15	300	310	320	330
c ($J K^{-1} g^{-1}$)	2.00	2.01	2.03	2.03	2.05	2.07	2.09
C ($J K^{-1} mol^{-1}$)	146	147	148	148	150	151	153
Temp. (K)	340	350	360	370	380	390	400
c ($J K^{-1} g^{-1}$)	2.11	2.14	2.16	2.19	2.22	2.26	2.29
C ($J K^{-1} mol^{-1}$)	154	156	158	160	163	165	167
Temp. (K)	410	420					
c ($J K^{-1} g^{-1}$)	2.33	2.36					
C ($J K^{-1} mol^{-1}$)	170	173					

TABLE 62.16.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	37	19	2.595	1.81–1	1.02	2.62–3	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
212.6–423.2	660.00	–2.80919	1.46233	1.30140+1	1.34914		V



Name: Ethyl ester carbamic acid
Formula: $C_3H_7NO_2$

CAS–RN: 51–79–6
Group No.: 62–017
Molar Mass: 89.09

TABLE 62.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
83DEW/DEK	325.8–336.3	4	nosp	99.94	melpt	C_p	BSAO	79SCH/OFF

TABLE 62.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.023	2.93–3	0.01	4.77–7	–1
Temp. range K		A_1	A_2				Level of uncertainty
325.8–336.3		1.70844+1	2.39352				III

TABLE 62.17.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p (J K^{-1}g^{-1})	2.331	2.354
C_p (J K^{-1}mol^{-1})	207.7	209.7

Name: 1–Methylethyl ester nitric acid
Formula: $C_3H_7NO_3$

CAS–RN: 1712–64–7
Group No.: 62–018
Molar Mass: 105.09

TABLE 62.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
88BUN	349.6	1	nosp	not specified		C_p	DDCT	85WAD
88LUS/RUB	191.5–300.0	39	0.05	98.72	melpt	C_p	BDAO	88LUS/RUB

TABLE 62.18.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88LUS/RUB	191.5–300.0	39	0.30#	0.738	4.90–2	0.22	2.21–4	–2

TABLE 62.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	40	39	0.768	5.10–2	0.23	2.21–4	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
191.5–300.0		2.28372+1	–4.04710	1.37152			III

TABLE 62.18.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.600	1.613	1.628	1.644	1.663	1.684	1.708
C_p (J K^{-1}mol^{-1})	168.2	169.5	171.0	172.8	174.8	177.0	179.5
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	1.733	1.742	1.761	1.791	1.817	1.823	
C_p (J K^{-1}mol^{-1})	182.2	183.0	185.1	188.2	190.9	191.6	

Name: 4–Oxobutanenitrile
Formula: C_4H_5NO

CAS–RN: 3515–93–3
Group No.: 62–019
Molar Mass: 83.09

TABLE 62.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
79DZH/KAR	N	210.0–320.0	12S	0.20	not specified	C_p	BSAO	54STR/ICK
81MUS/GAN	N	220.0–370.0	12	0.50	not specified	C_p	BSAO	54STR/ICK

79DZH/KAR above 320 K sample decomposes and polymerizes probably due to impurities
81MUS/GAN calorimeter adapted for continuous heating

TABLE 62.19.2. Correlated heat capacities

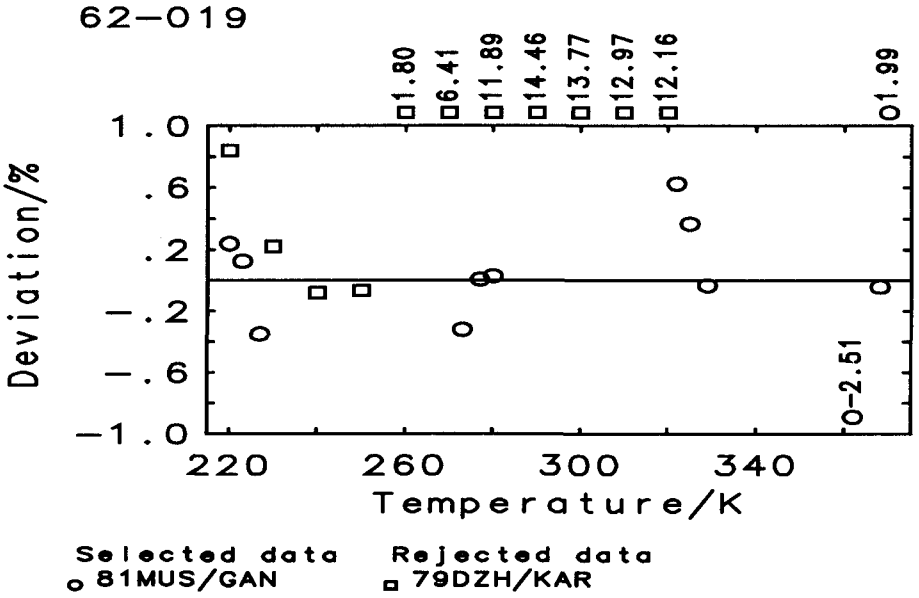
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
81MUS/GAN	220.0–370.0	12	0.50	1.924	2.11–1	0.96	4.13–3	1
				Rejected data				
79DZH/KAR	(2.11, 9.05, 1.56, 7)							

TABLE 62.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	12	2.357	2.59–1	1.18	4.13–3	1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
220.0–370.0	–2.99011+1	5.20027+1	–1.83037+1	2.18320			V

TABLE 62.19.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.92	1.95	1.97	1.98	2.00	2.01	2.01
C_p (J K^{-1}mol^{-1})	159	162	163	165	166	167	167
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	2.01	2.02	2.03	2.03	2.05	2.06	2.09
C_p (J K^{-1}mol^{-1})	167	168	169	169	170	171	173
Temp. (K)	340	350	360	370			
c_p (J K^{-1}g^{-1})	2.11	2.15	2.20	2.25			
C_p (J K^{-1}mol^{-1})	176	179	183	187			



Name: 2,5–Pyrrolidinedione
Formula: $C_4H_5NO_2$

CAS–RN: 123–56–8
Group No.: 62–020
Molar Mass: 99.09

TABLE 62.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89STE/CHI3	405.0–495.0	10	1.00	99.95	chrom	C_{sat}	BDHT	89KNI/ARC

TABLE 62.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.044	1.13–2	0.04	5.53–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
405.0–495.0		1.33747+1	2.64706				IV

TABLE 62.20.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450	460
c_{sat} (J K^{-1}g^{-1})	2.011	2.033	2.055	2.077	2.100	2.122	2.144
C_{sat} (J K^{-1}mol^{-1})	199.2	201.4	203.6	205.8	208.0	210.2	212.4
Temp. (K)	470	480	490	500			
c_{sat} (J K^{-1}g^{-1})	2.166	2.188	2.211	2.233			
C_{sat} (J K^{-1}mol^{-1})	214.6	216.8	219.0	221.2			

Name: 3-Methoxypropionitrile
Formula: C_4H_7NO

CAS-RN: 110-67-8
Group No.: 62-021
Molar Mass: 85.11

TABLE 62.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91SVO/ZAB1	300.6–328.4	7	0.30	99.96	chrom	C_p	BSAO	91SVO/ZAB1

TABLE 62.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.140	9.15-3	0.04	7.36-6	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
300.6–328.4		4.70937+1	-1.68548+1	2.79854			III

TABLE 62.21.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330
c_p (J K^{-1}g^{-1})	2.122	2.124	2.131	2.144
C_p (J K^{-1}mol^{-1})	180.6	180.7	181.4	182.5

Name: 2-Pyrrolidinone
Formula: C_4H_7NO

CAS-RN: 616-45-5
Group No.: 62-022
Molar Mass: 85.11

TABLE 62.22.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62KOL/PAU	N	300.0–350.0	10S	nosp	99.88	melpt	C_p	BSAO	56POP/KOL
89STE/CHI3		300.0	1	1.00	99.99	chrom	C_p	BDHT	89KNI/ARC

62KOL/PAU some data in 59KOL/PAU

TABLE 62.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62KOL/PAU	300.0–350.0	10	0.70#	0.019	2.85–3	0.01	–1.25–3	–4
89STE/CHI3	300.0	1	1.00	0.126	2.57–2	0.13	2.57–2	1

TABLE 62.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.047	9.08–3	0.04	1.20–3	–3

Temp. range K	A_1	A_2	Level of uncertainty
300.0–350.0	5.65623	4.90587	IV

TABLE 62.22.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p ($J K^{-1} g^{-1}$)	1.990	2.038	2.086	2.134	2.182	2.230
C_p ($J K^{-1} mol^{-1}$)	169.4	173.5	177.6	181.6	185.7	189.8

Name: 2–Butanone oxime
Formula: C_4H_9NO

CAS–RN: 96–29–7
Group No.: 62–023
Molar Mass: 87.12

TABLE 62.23.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
02LOU2	N	359.84	2.721	nosp	not specified		C_{avg}	DSIO	*98LOU

02LOU2 average value in temperature range 295–425 K

Name: *N*,*N*–Dimethylacetamide
Formula: C_4H_9NO

CAS–RN: 127–19–5
Group No.: 62–024
Molar Mass: 87.12

TABLE 62.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73MOS/NIK	254.1–298.1	3S	nosp	98.5	melpt	C_p	BSAO	66NIK/LEB
78DEV/HEU	298.1	1	1.00	99.8	chrom	C_p	BSIO	70LKB/COM
84ZEG/SOM1	298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED
91OGA/MIT	298.1	1	nosp	not specified		C_p	FSIO	85OGA

TABLE 62.24.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73MOS/NIK	254.1–298.1	3	0.50#	1.930	2.05–1	0.97	1.36–1	1
78DEV/HEU	298.1	1	1.00	1.783	3.82–1	1.78	3.82–1	1
84ZEG/SOM1	298.1	1	0.50#	0.146	1.54–2	0.07	1.54–2	1
91OGA/MIT	298.1	1	0.30#	2.847	1.78–1	0.85	–1.78–1	–1

TABLE 62.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	2.371	2.76–1	1.29	1.05–1	2
Temp. range K		A_1	A_2				Level of uncertainty
254.1–298.1		1.85781+1	8.29161–1				V

TABLE 62.24.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.98	1.99	1.99	1.99	2.00	2.01	2.01
C_p ($J K^{-1} mol^{-1}$)	172	173	173	174	174	175	175

Name: *N*–Ethylacetamide
Formula: C_4H_9NO

CAS–RN: 625–50–3
Group No.: 62–025
Molar Mass: 87.12

TABLE 62.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM
86ZEG/BOE	298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED

TABLE 62.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71KON/WAD	298.1	1	0.50#	0.155	1.68–2	0.08	–1.68–2	–1
86ZEG/BOE	298.1	1	0.50#	0.156	1.69–2	0.08	1.69–2	1

TABLE 62.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.220	2.38–2	0.11	2.67–5	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		2.16657+1					III

TABLE 62.25.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.068
C_p (J K^{-1}mol^{-1})	180.1

Name: *N*–Methylpropanamide
Formula: C_4H_9NO

CAS–RN: 1187–58–2
Group No.: 62–026
Molar Mass: 87.12

TABLE 62.26.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71KON/WAD	298.15	2.055	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: Morpholine
Formula: C_4H_9NO

CAS–RN: 110–91–8
Group No.: 62–027
Molar Mass: 87.12

TABLE 62.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
42TRI/ENG	N	273.0–403.0	eqn	nosp	not specified		C_p	DSIO	38FRE/HIL1
80LYA		293.0–353.0	eqn	0.80	not specified		C_p	BSIO	49WEI

42TRI/ENG calculated from temperature dependence of enthalpy by the compilers

TABLE 62.27.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
42TRI/ENG	273.0–402.6	13	1.00#	0.000	9.16–7	0.00	4.40–7	0
				Rejected data				
80LYA	(6.89–1, 3.45,–4.10–1, –2)							

TABLE 62.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	13	0.000	1.04–6	0.00	4.40–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
273.0–402.6		2.97928+1	–7.05163	1.36784			V

TABLE 62.27.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J K^{-1} g^{-1}$)	1.98	1.98	1.98	1.99	2.00	2.00	2.01
C_p ($J K^{-1} mol^{-1}$)	172	172	173	173	174	174	175
Temp. (K)	320	330	340	350	360	370	380
c_p ($J K^{-1} g^{-1}$)	2.03	2.04	2.06	2.09	2.11	2.14	2.17
C_p ($J K^{-1} mol^{-1}$)	177	178	180	182	184	186	189
Temp. (K)	390	400					
c_p ($J K^{-1} g^{-1}$)	2.20	2.24					
C_p ($J K^{-1} mol^{-1}$)	192	195					

Name: 2–Amino–2–methyl–1–propanol
Formula: $C_4H_{11}NO$

CAS–RN: 124–68–5
Group No.: 62–028
Molar Mass: 89.14

TABLE 62.28.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80ROU/ROB	298.15	2.575	0.30	not specified		C_p	FSIT	71PIC/LED

Name: *N*,*N*–Diethylhydroxylamine
Formula: $C_4H_{11}NO$

CAS–RN: 3710–84–7
Group No.: 62–029
Molar Mass: 89.14

TABLE 62.29.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
90STE/CHI	N	298.15	4.160	nosp	99.92	chrom	C_p	BDHT	89KNI/ARC

90STE/CHI too high value C_p, probably misprint

Name: 3–Methoxy–1–propanamine
Formula: $C_4H_{11}NO$

CAS–RN: 5332–73–0
Group No.: 62–030
Molar Mass: 89.14

TABLE 62.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84GEI/KAR	200.0–300.0	13S	0.30	99.7	chrom	C_p	BSAO	54STR/ICK

TABLE 62.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.318	2.49–2	0.10	3.99–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
200.0–300.0	2.29587+1	1.39868	III

TABLE 62.30.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J\,K^{-1}g^{-1}$)	2.402	2.416	2.429	2.442	2.455	2.468	2.481
C_p ($J\,K^{-1}mol^{-1}$)	214.1	215.3	216.5	217.6	218.8	220.0	221.1
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J\,K^{-1}g^{-1}$)	2.494	2.498	2.507	2.520	2.531	2.533	
C_p ($J\,K^{-1}mol^{-1}$)	222.3	222.7	223.5	224.6	225.6	225.8	

Name: 2–Amino–2–methyl–1,3–propanediol
Formula: $C_4H_{11}NO_2$

CAS–RN: 115–69–5
Group No.: 62–031
Molar Mass: 105.14

TABLE 62.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89ZHA/YAN1	N	387.7–393.6	3	nosp	not specified		C_p	BSAO	88ZHA/ZOU

89ZHA/YAN1 experimental values provided by the authors

TABLE 62.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.597	2.44–1	0.60	9.68–4	–1

Temp. range K	A_1	A_2	Level of uncertainty
387.7–393.6	9.53256	8.02290	V

TABLE 62.31.4. Recommended values of heat capacities

Temp. (K)	385	395
c_p (J K^{-1}g^{-1})	3.20	3.26
C_p (J K^{-1}mol^{-1})	336	343

Name: 2–Amino–2–(hydroxymethyl)–1,3–propanediol
Formula: $C_4H_{11}NO_3$

CAS–RN: 77–86–1
Group No.: 62–032
Molar Mass: 121.14

TABLE 62.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90ZHA/YAN	445.8–450.6	2	nosp	not specified		C_p	BSAO	88ZHA/ZOU

TABLE 62.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	1.53–5	0

Temp. range K	A_1	A_2	Level of uncertainty
445.8–450.6	–1.67961+2	4.92084+1	IV

TABLE 62.32.4. Recommended values of heat capacities

Temp. (K)	445	450
c_p (J K^{-1}g^{-1})	3.502	3.671
C_p (J K^{-1}mol^{-1})	424.2	444.6

Name: Ethyl ester cyanoacetic acid
Formula: $C_5H_7NO_2$

CAS–RN: 105–56–6
Group No.: 62–033
Molar Mass: 113.12

TABLE 62.33.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87KHO/BUG	N	251.4–298.4	16	1.00	not specified		C_p	BSAO	87KHO/BUG

87KHO/BUG smoothed data in 91ISK/ISM

TABLE 62.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	16	0.355	9.35–2	0.36	5.81–4	2
Temp. range K		A_1	A_2				Level of uncertainty
251.4–298.4		2.17953+1	1.60750				V

TABLE 62.33.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.90	1.91	1.92	1.92	1.93	1.94	1.95
C_p (J K^{-1}mol^{-1})	215	216	217	218	219	220	221
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.96						
C_p (J K^{-1}mol^{-1})	221						

Name: 1–Methyl–2–pyrrolidinone
Formula: C_5H_9NO

CAS–RN: 872–50–4
Group No.: 62–034
Molar Mass: 99.13

TABLE 62.34.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78MAR/CIO1	N	298.1–470.0	19S	nosp	not specified		C_p	DSIO	71MAR/CIO
89VAS/NOV	N	288.0–323.0	4	0.50	not specified		C_p	BSIO	89VAS/NOV
90STE/CHI	N	298.1	1	nosp	99.	chrom	C_p	BDHT	89KNI/ARC

78MAR/CIO1 values calculated from temperature dependence of enthalpy by the authors; suspect values
89VAS/NOV water content 0.02 weight %
90STE/CHI too high value C_p, probably misprint

TABLE 62.34.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89VAS/NOV	288.0–323.0	4	0.50	0.449	4.74–2	0.22	2.19–4	2
				Rejected data				
78MAR/CIO1	(1.23+1, 35.35, 1.15+1, 4)			90STE/CHI	(2.87+1, 57.87, 2.87+1, 1)			

TABLE 62.34.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	4	0.635	6.71–2	0.32	2.19–4	2
Temp. range K		A_1	A_2				Level of uncertainty
288.0–323.0		1.41243+1	2.27149				VI

TABLE 62.34.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	1.74	1.75	1.76	1.78	1.79
C_p ($J K^{-1}mol^{-1}$)	172	174	174	176	178

Name: 2–Piperidinone
Formula: C_5H_9NO

CAS–RN: 675–20–7
Group No.: 62–035
Molar Mass: 99.13

TABLE 62.35.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62KOL/PAU	N	320.0–350.0	7S	nosp	99.0	melpt	C_p	BSAO	56POP/KOL

62KOL/PAU some data in 59KOL/PAU

TABLE 62.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.009	1.65–3	0.01	1.09–6	0
Temp. range K		A_1	A_2				Level of uncertainty
320.0–350.0		4.23986	6.72468				IV

TABLE 62.35.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	2.160	2.217	2.273	2.330
C_p ($J K^{-1}mol^{-1}$)	214.2	219.8	225.4	230.9

Name: *N*,2–Dimethylpropanamide
Formula: $C_5H_{11}NO$

CAS–RN: 2675–88–9
Group No.: 62–036
Molar Mass: 101.15

TABLE 62.36.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.15	2.066	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: *N*–Methylbutanamide
Formula: $C_5H_{11}NO$

CAS–RN: 17794–44–4
Group No.: 62–037
Molar Mass: 101.15

TABLE 62.37.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.15	2.046	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: *N*–(1–Methylethyl)acetamide
Formula: $C_5H_{11}NO$

CAS–RN: 1118–69–0
Group No.: 62–038
Molar Mass: 101.15

TABLE 62.38.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.15	2.086	nosp	99.8	chrom	C_p	BSIO	70LKB/COM

Name: *N*–Propylacetamide
Formula: $C_5H_{11}NO$

CAS–RN: 5331–48–6
Group No.: 62–039
Molar Mass: 101.15

TABLE 62.39.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM
86ZEG/BOE	298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED

TABLE 62.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
71KON/WAD	298.1	1	0.50#	0.452	5.63–2	0.23	–5.63–2	–1
86ZEG/BOE	298.1	1	0.50#	0.454	5.68–2	0.23	5.68–2	1

TABLE 62.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.641	7.99–2	0.32	2.56–4	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		2.49525+1					III

TABLE 62.39.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	2.051
C_p (J K^{-1}mol^{-1})	207.5

Name: Tetramethylurea
Formula: $C_5H_{12}N_2O$

CAS–RN: 632–22–4
Group No.: 62–040
Molar Mass: 116.16

TABLE 62.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88KOZ/KRA	320.0–425.0	eqn	2.00	not specified		C_p	BDHT	92KAB/KOZ

TABLE 62.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	11	11	0.000	1.68–6	0.00	8.67–7	0
Temp. range K		A_1	A_2				Level of uncertainty
320.0–425.0		1.84377+1	3.30506				V

TABLE 62.40.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350	360	370	380
c_p (J K^{-1}g^{-1})	2.08	2.10	2.12	2.15	2.17	2.19	2.22
C_p (J K^{-1}mol^{-1})	241	244	247	249	252	255	258
Temp. (K)	390	400	410	420	430		
c_p (J K^{-1}g^{-1})	2.24	2.27	2.29	2.31	2.34		
C_p (J K^{-1}mol^{-1})	260	263	266	269	271		

Name: 2-(Ethylmethylamino)ethanol
Formula: $C_5H_{13}NO$

CAS-RN: 2893-43-8
Group No.: 62-041
Molar Mass: 103.16

TABLE 62.41.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEB/RYA	N	320.5–340.5	2	1.00	99.8	chrom	C_{avg}	DSIO	76LEB/RYA

81LEB/RYA average values in temperature ranges 298–343 K and 298–383 K

TABLE 62.41.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
320.5–340.5		3.51733	8.53929				V

TABLE 62.41.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J\,K^{-1}g^{-1}$)	2.49	2.55	2.62
C ($J\,K^{-1}mol^{-1}$)	256	264	271

Name: 1,2-Dinitrobenzene
Formula: $C_6H_4N_2O_4$

CAS-RN: 528-29-0
Group No.: 62-042
Molar Mass: 168.11

TABLE 62.42.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	390.0–513.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.000	2.04–6	0.00	8.48–7	0
Temp. range K		A_1	A_2				Level of uncertainty
390.0–513.2		2.18263+1	2.81801				VI

TABLE 62.42.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	1.62	1.64	1.65	1.66	1.68	1.69	1.71
C_p ($J K^{-1} mol^{-1}$)	273	275	278	280	282	285	287
Temp. (K)	460	470	480	490	500	510	
c_p ($J K^{-1} g^{-1}$)	1.72	1.73	1.75	1.76	1.78	1.79	
C_p ($J K^{-1} mol^{-1}$)	289	292	294	296	299	301	

Name: 1,3–Dinitrobenzene
Formula: $C_6H_4N_2O_4$

CAS–RN: 99–65–0
Group No.: 62–043
Molar Mass: 168.11

TABLE 62.43.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	363.2–518.2	2	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN constant value calculated from temperature dependence of enthalpy by the authors

TABLE 62.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
363.2–518.2		3.43194+1					VI

TABLE 62.43.4. Recommended values of heat capacities

Temp. (K)	370	420	470	520
c_p ($J K^{-1} g^{-1}$)	1.70	1.70	1.70	1.70
C_p ($J K^{-1} mol^{-1}$)	285	285	285	285

Name: 1,4–Dinitrobenzene
Formula: $C_6H_4N_2O_4$

CAS–RN: 100–25–4
Group No.: 62–044
Molar Mass: 168.11

TABLE 62.44.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	446.0–483.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	3	3	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
446.0–483.0		8.36362	5.58571				VI

TABLE 62.44.4. Recommended values of heat capacities

Temp. (K)	450	460	470	480
c_p ($J K^{-1} g^{-1}$)	1.66	1.68	1.71	1.74
C_p ($J K^{-1} mol^{-1}$)	279	283	288	292

Name: Nitrobenzene
Formula: $C_6H_5NO_2$

CAS-RN: 98–95–3
Group No.: 62–045
Molar Mass: 123.11

TABLE 62.45.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
*81VON	323.4–392.1	4S	nosp	not specified		C_{avg}	DSIO	*81VON
12SCH2	283.1–393.1	12	nosp	not specified		C_p	BSIO	12SCH1
24WIL/DAN	303.0–358.0	eqn	nosp	not specified		C_p	BSAO	24WIL/DAN
34PAR/TOD	280.6–297.4	5	0.60	not specified		C_p	BSIO	25PAR
36PAR/TOD1	280.0–300.0	3S	0.70	not specified		C_p	BSIO	25PAR
39MAZ1	278.5–293.4	50	nosp	not specified		C_p	BSIO	39MAZ3
39MAZ3	279.0–293.4	10	nosp	not specified		C_p	BSIO	39MAZ3
58LUT/PAN	335.6–414.6	15	0.70	not specified		C_p	BDHO	58LUT/PAN
67PAC	303.1	1	nosp	not specified		C_p	BDHT	79DU/COM
67RAS/GAN	293.1–373.1	5S	0.50	not specified		C_p	BSAO	67RAS/GAN
85LAI/ROD	298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED

TABLE 62.45.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
39MAZ1	278.5–293.4	50	0.70#	0.068	1.01–2	0.05	1.93–4	–3
39MAZ3	279.0–293.4	10	0.70#	0.211	3.16–2	0.15	–4.16–3	–4
58LUT/PAN	335.6–414.6	15	0.70	1.191	2.06–1	0.83	–3.17–2	–5
67RAS/GAN	293.1–373.1	5	0.50	0.786	9.04–2	0.39	5.39–2	3
85LAI/ROD	298.1	1	0.50#	0.176	1.92–2	0.09	1.92–2	1
				Rejected data				
*81VON	(2.23–1, 0.95, 1.42–1, 2)			12SCH2	(1.78, 8.50,–1.45, –10)			
24WIL/DAN	(5.67–1, 2.57,–5.67–1, –3)			34PAR/TOD	(5.91–1, 2.67, 5.87–1, 5)			
36PAR/TOD1	(6.13–1, 2.76, 6.08–1, 3)			67PAC	(8.40–1, 3.99,–8.40–1, –1)			

TABLE 62.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	109	81	0.571	9.47–2	0.39	–2.71–3	–8
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
278.5–414.6		–4.67776+1	5.99271+1	–1.80107+1	1.88554		IV

TABLE 62.45.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	1.432	1.454	1.470	1.473	1.492	1.509	1.527
C_p (J K^{-1}mol^{-1})	176.3	179.0	181.0	181.4	183.6	185.8	188.0
Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	1.545	1.565	1.588	1.614	1.643	1.678	1.718
C_p (J K^{-1}mol^{-1})	190.2	192.7	195.5	198.7	202.3	206.6	211.5
Temp. (K)	410						
c_p (J K^{-1}g^{-1})	1.764						
C_p (J K^{-1}mol^{-1})	217.2						

TABLE 62.45.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	109	81	0.699	1.07–1	0.46	–9.39–3	6
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
278.5–414.6	718.00	1.32777+1	1.26993+1	5.64869	3.47061		IV

Name: 2–Nitrophenol
Formula: $C_6H_5NO_3$

CAS–RN: 88–75–5
Group No.: 62–046
Molar Mass: 139.11

TABLE 62.46.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
16KUR	N	430.6	1	nosp	not specified	C_{avg}	not specified	
59LUT/PAN		335.0–409.0	eqn	nosp	not specified	C_p	BDHO	58LUT/PAN

16KUR average value in temperature range 413–448 K

TABLE 62.46.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59LUT/PAN	335.0–409.4	9	3.00#	0.000	1.10–6	0.00	2.12–7	0

TABLE 62.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	9	0.000	1.35–6	0.00	2.12–7	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
335.0–409.4		4.53459+1	–1.57990+1	3.23414			V

TABLE 62.46.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	1.73	1.77	1.82	1.86	1.91	1.97	2.03
C_p (J K^{-1}mol^{-1})	241	247	253	259	266	274	282
Temp. (K)	410						
c_p (J K^{-1}g^{-1})	2.09						
C_p (J K^{-1}mol^{-1})	290						

Name: 3–Nitrophenol
Formula: $C_6H_5NO_3$

CAS–RN: 554–84–7
Group No.: 62–047
Molar Mass: 139.11

TABLE 62.47.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
16KUR	N	433.1	1	nosp	not specified		C_{avg}	not specified	
35SKA	N	370.0–380.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN
59LUT/PAN		378.0–408.0	eqn	nosp	not specified		C_p	BDHO	58LUT/PAN

16KUR average value in temperature range 418–448 K
35SKA temperature range not specified, recommended use near n.m.t.

TABLE 62.47.2. Correlated heat capacities

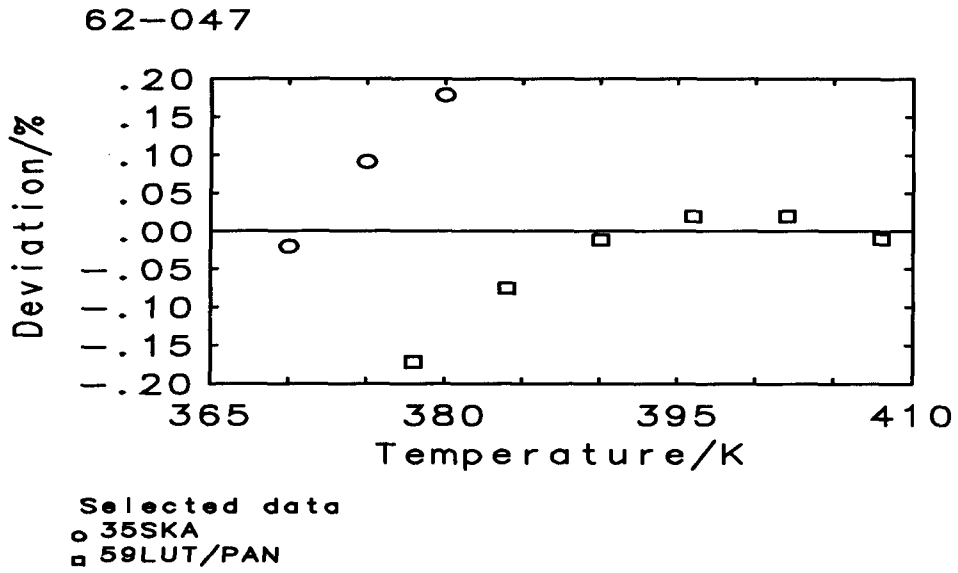
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
35SKA	370.0–380.0	3	3.00#	0.037	3.42–2	0.11	3.28–2	3
59LUT/PAN	378.0–408.0	6	3.00#	0.035	3.23–2	0.11	–1.63–2	–2

TABLE 62.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	9	0.041	3.73–2	0.12	7.67–5	1
Temp. range K		A_1	A_2				Level of uncertainty
370.0–408.0		1.10918+1	5.11128				V

TABLE 62.47.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410
c_p ($J K^{-1} g^{-1}$)	1.79	1.82	1.85	1.88	1.92
C_p ($J K^{-1} mol^{-1}$)	249	254	258	262	266



Name: 4–Nitrophenol
Formula: $C_6H_5NO_3$

CAS–RN: 100–02–7
Group No.: 62–048
Molar Mass: 139.11

TABLE 62.48.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
16KUR	N	435.6	1	nosp	not specified	C_{avg}	not specified	
59LUT/PAN		391.0–410.0	eqn	nosp	not specified	C_p	BDHO	58LUT/PAN

16KUR average value in temperature range 423–448 K

TABLE 62.48.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59LUT/PAN	391.0–410.2	5	3.00#	0.000	1.91–6	0.00	–1.14–6	0

TABLE 62.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	5	0.000	2.46–6	0.00	–1.14–6	0
Temp. range K		A_1	A_2				Level of uncertainty
391.0–410.2		9.78957	5.56523				V

TABLE 62.48.4. Recommended values of heat capacities

Temp. (K)	390	400	410
c_p ($J K^{-1} g^{-1}$)	1.88	1.92	1.95
C_p ($J K^{-1} mol^{-1}$)	262	266	271

Name: 2–Nitrobenzenamine
Formula: $C_6H_6N_2O_2$

CAS–RN: 88–74–4
Group No.: 62–049
Molar Mass: 138.13

TABLE 62.49.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	343.0–423.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	2.34–6	0.00	1.27–6	0
Temp. range K		A_1	A_2				Level of uncertainty
343.0–423.0		1.58171+1	4.40818				VI

TABLE 62.49.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1}g^{-1}$)	1.88	1.91	1.93	1.96	1.99	2.01	2.04
C_p ($J K^{-1}mol^{-1}$)	260	263	267	271	274	278	282
Temp. (K)	420						
c_p ($J K^{-1}g^{-1}$)	2.07						
C_p ($J K^{-1}mol^{-1}$)	285						

Name: 3–Nitrobenzenamine
Formula: $C_6H_6N_2O_2$

CAS–RN: 99–09–2
Group No.: 62–050
Molar Mass: 138.13

TABLE 62.50.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	385.0–483.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.000	3.08–6	0.00	1.91–6	0
Temp. range K		A_1	A_2				Level of uncertainty
385.0–482.8		1.62780+1	4.02573				VI

TABLE 62.50.4. Recommended values of heat capacities

Temp. (K)	390	400	410	420	430	440	450
c_p ($J K^{-1}g^{-1}$)	1.92	1.95	1.97	2.00	2.02	2.05	2.07
C_p ($J K^{-1}mol^{-1}$)	266	269	273	276	279	283	286
Temp. (K)	460	470	480				
c_p ($J K^{-1}g^{-1}$)	2.09	2.12	2.14				
C_p ($J K^{-1}mol^{-1}$)	289	293	296				

Name: 4–Nitrobenzenamine
Formula: $C_6H_6N_2O_2$

CAS–RN: 100–01–6
Group No.: 62–051
Molar Mass: 138.13

TABLE 62.51.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	421.0–468.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.000	2.04–6	0.00	8.48–7	0
Temp. range K		A_1	A_2				Level of uncertainty
421.0–468.2		2.30920+1	2.41544				VI

TABLE 62.51.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470
c_p (J K^{-1}g^{-1})	2.00	2.02	2.03	2.04	2.06	2.07
C_p (J K^{-1}mol^{-1})	276	278	280	282	284	286

Name: Cyclohexanone oxime
Formula: $C_6H_{11}NO$

CAS-RN: 100-64-1
Group No.: 62-052
Molar Mass: 113.16

TABLE 62.52.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
91KOZ/SHE	N	380.0–430.0	eqn	2.00	not specified	C_p	BDHT	92KAB/KOZ

91KOZ/SHE same equation in 92KOZ/KAB

TABLE 62.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
380.0–430.0		2.57742+1	2.28516				V

TABLE 62.52.4. Recommended values of heat capacities

Temp. (K)	380	390	400	410	420	430
c_p (J K^{-1}g^{-1})	2.53	2.55	2.57	2.58	2.60	2.62
C_p (J K^{-1}mol^{-1})	286	288	290	292	294	296

Name: Hexahydro–2H–azepin–2–one
Formula: $C_6H_{11}NO$

CAS–RN: 105–60–2
Group No.: 62–053
Molar Mass: 113.16

TABLE 62.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62KOL/PAU	N	345.0–375.0	7S	nosp	99.95	melpt	C_p	BSAO	56POP/KOL
89KOZ/MAR		350.0–510.0	eqn	1.50	99.95	anal	C_p	BDHT	92KAB/KOZ
92KAB/KOZ	N	342.0–520.0	eqn	1.50	not specified		C_p	BDHT	92KAB/KOZ

62KOL/PAU some data in 59KOL/PAU and 59PAU/KOL
92KAB/KOZ same equation in 91KOZ/SHE

TABLE 62.53.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62KOL/PAU	345.0–375.0	7	0.80#	1.241	3.02–1	0.99	1.01–1	1
89KOZ/MAR	350.0–509.6	15	1.50	0.417	1.90–1	0.62	–1.54–1	–12
				Rejected data				
92KAB/KOZ	(8.45, 20.83, 8.33, 13)							

TABLE 62.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	22	0.818	2.43–1	0.80	–7.27–2	–11
Temp. range K		A_1	A_2				Level of uncertainty
345.0–509.6		1.78776+1	3.34580				V

TABLE 62.53.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1}g^{-1}$)	2.17	2.20	2.22	2.25	2.27	2.30	2.32
C_p ($J K^{-1}mol^{-1}$)	246	249	252	254	257	260	263
Temp. (K)	420	430	440	450	460	470	480
c_p ($J K^{-1}g^{-1}$)	2.35	2.37	2.40	2.42	2.44	2.47	2.49
C_p ($J K^{-1}mol^{-1}$)	265	268	271	274	277	279	282
Temp. (K)	490	500	510				
c_p ($J K^{-1}g^{-1}$)	2.52	2.54	2.57				
C_p ($J K^{-1}mol^{-1}$)	285	288	291				

Name: 4,4–Dimethoxybutanenitrile
Formula: $C_6H_{11}NO_2$

CAS–RN: 14618–78–1
Group No.: 62–054
Molar Mass: 129.16

TABLE 62.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83GEI/KAR	154.0–300.0	18S	0.30	99.8	chrom	C_p	BSAO	54STR/ICK

TABLE 62.54.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	18	0.317	2.77–2	0.09	3.81–5	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
154.0–230.0	3.92845+1	–1.51426+1	7.08727	–1.05796	IV
230.0–300.0	–1.49704+1	5.56246+1	–2.36811+1	3.40122	IV

TABLE 62.54.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.872	1.876	1.882	1.889	1.901	1.905	1.917
C_p (J K^{-1}mol^{-1})	241.8	242.3	243.0	244.0	245.5	246.1	247.6

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	1.940	1.964	1.970
C_p (J K^{-1}mol^{-1})	250.6	253.7	254.5

Name: *N*–Butylacetamide
Formula: $C_6H_{13}NO$

CAS–RN: 1119–49–9
Group No.: 62–055
Molar Mass: 115.18

TABLE 62.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM
86ZEG/BOE	298.1	1	nosp	99.5	chrom	C_p	FSIT	71PIC/LED

TABLE 62.55.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
71KON/WAD	298.1	1	0.50#	0.376	5.33–2	0.19	–5.33–2	–1
86ZEG/BOE	298.1	1	0.50#	0.377	5.37–2	0.19	5.37–2	1

TABLE 62.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.532	7.57–2	0.27	2.01–4	0
Temp. range K		A_1					Level of uncertainty
298.1–298.1		2.84374+1					III

TABLE 62.55.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J\,K^{-1}g^{-1}$)	2.053
C_p ($J\,K^{-1}mol^{-1}$)	236.4

Name: *N*,*N*–Diethylacetamide
Formula: $C_6H_{13}NO$

CAS–RN: 685–91–6
Group No.: 62–056
Molar Mass: 115.18

TABLE 62.56.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
84ZEG/SOM1	298.15	2.089	0.30	99.5	chrom	C_p	FSIT	71PIC/LED

Name: *N*–Methylpentanamide
Formula: $C_6H_{13}NO$

CAS–RN: 6225–10–1
Group No.: 62–057
Molar Mass: 115.18

TABLE 62.57.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71KON/WAD	298.1	1	nosp	99.8	chrom	C_p	BSIO	70LKB/COM
76SKO/SUU	298.1	1	0.10	not specified		C_p	DDCT	71KON/SUU

TABLE 62.57.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
76SKO/SUU	298.1	1	0.10	0.000	0.00	0.00	0.00	0
				Rejected data				
71KON/WAD	(1.13, 4.11,–1.13, –1)							

TABLE 62.57.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	1	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
298.1–298.1	2.86728+1	III

TABLE 62.57.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p ($J\,K^{-1}g^{-1}$)	2.070
C_p ($J\,K^{-1}mol^{-1}$)	238.4

Name: Dipropyldiazene 1–oxide
Formula: $C_6H_{14}N_2O$

CAS–RN: 17697–55–1
Group No.: 62–058
Molar Mass: 130.19

TABLE 62.58.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81BYS	N	298.15	2.000	nosp	100.0	chrom	C_p	BDHT	69PER/COM

81BYS correction for water content (0.017 mass %)

Name: 2,2',2''–Nitrilotrisethanol
Formula: $C_6H_{15}NO_3$

CAS–RN: 102–71–6
Group No.: 62–059
Molar Mass: 149.19

TABLE 62.59.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
34MEH1		290.1	1	1.50	not specified		C_p	BSIO	49WEI
82MIN/SAB	N	298.1	1	nosp	99.	anal	C_p	not specified	

82MIN/SAB thermopile conduction calorimeter (Tian–Calvet) used but, not described

TABLE 62.59.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
			Selected data					
34MEH1	290.1	1	1.50	0.000	3.82–6	0.00	–3.82–6	0
82MIN/SAB	298.1	1	1.00#	0.000	3.82–6	0.00	–3.82–6	0

TABLE 62.59.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	–3.82–6	0
Temp. range K		A_1	A_2				Level of uncertainty
290.1–298.1		–2.81668+1	2.51548+1				V

TABLE 62.59.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	2.50	2.61	2.64
C_p ($J K^{-1} mol^{-1}$)	372	389	393

Name: Benzoxazole
Formula: C_7H_5NO

CAS–RN: 273–53–0
Group No.: 62–060
Molar Mass: 119.12

TABLE 62.60.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
92STE/CHI2	308.9–437.4	13	0.10	99.963	melpt	C_{sat}	BSAO	47HUF
92STE/CHI2	320.0–660.0	18	nosp	99.963	melpt	C_{sat}	BDHT	89KNI/ARC

TABLE 62.60.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
92STE/CHI2	308.9–437.4	13	0.10	0.240	5.67–3	0.02	–2.02–4	1
92STE/CHI2	320.0–660.0	18	1.00#	0.167	5.53–2	0.17	1.50–2	11

TABLE 62.60.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	31	0.224	4.71–2	0.14	8.64–3	12
C_{sat}	31	31	0.214	3.67–2	0.12	9.16–3	11
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
308.9–450.0		1.30079+1	2.23129	2.37734–1	–1.18038–2		II
450.0–580.0		4.30458	8.03350	–1.05164	8.37057–2		III
580.0–660.0		–1.27653+3	6.70535+2	–1.15276+2	6.64832		IV
308.9–450.0		1.35348+1	1.76038	3.77524–1	–2.55814–2		II
450.0–580.0		1.01656+1	4.00652	–1.21618–1	1.13921–2		III
580.0–660.0		–7.01709+2	3.72218+2	–6.36063+1	3.65994		IV

TABLE 62.60.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p (J K^{-1}g^{-1})	1.526	1.549	1.573	1.597	1.621	1.645	1.670
C_p (J K^{-1}mol^{-1})	181.7	184.5	187.4	190.2	193.1	196.0	198.9
c_{sat} (J K^{-1}g^{-1})	1.526	1.549	1.573	1.597	1.621	1.645	1.670
C_{sat} (J K^{-1}mol^{-1})	181.7	184.5	187.4	190.2	193.1	196.0	198.9
Temp. (K)	380	390	400	410	420	430	440
c_p (J K^{-1}g^{-1})	1.694	1.719	1.744	1.769	1.794	1.819	1.844
C_p (J K^{-1}mol^{-1})	201.8	204.8	207.7	210.7	213.7	216.7	219.7
c_{sat} (J K^{-1}g^{-1})	1.694	1.719	1.744	1.768	1.793	1.818	1.843
C_{sat} (J K^{-1}mol^{-1})	201.8	204.7	207.7	210.7	213.6	216.6	219.6
Temp. (K)	450	460	470	480	490	500	510
c_p (J K^{-1}g^{-1})	1.870	1.895	1.921	1.947	1.973	1.999	2.026
C_p (J K^{-1}mol^{-1})	222.7	225.8	228.8	231.9	235.0	238.2	241.3
c_{sat} (J K^{-1}g^{-1})	1.869	1.894	1.919	1.944	1.970	1.995	2.020
C_{sat} (J K^{-1}mol^{-1})	222.6	225.6	228.6	231.6	234.6	237.6	240.7
Temp. (K)	520	530	540	550	560	570	580
c_p (J K^{-1}g^{-1})	2.053	2.080	2.108	2.136	2.165	2.194	2.223
C_p (J K^{-1}mol^{-1})	244.5	247.8	251.1	254.4	257.9	261.3	264.8
c_{sat} (J K^{-1}g^{-1})	2.046	2.072	2.097	2.123	2.149	2.175	2.201
C_{sat} (J K^{-1}mol^{-1})	243.7	246.8	249.8	252.9	256.0	259.1	262.2
Temp. (K)	590	600	610	620	630	640	650
c_p (J K^{-1}g^{-1})	2.254	2.288	2.328	2.377	2.438	2.513	2.606
C_p (J K^{-1}mol^{-1})	268.5	272.5	277.3	283.2	290.4	299.4	310.4
c_{sat} (J K^{-1}g^{-1})	2.228	2.256	2.287	2.323	2.365	2.415	2.474
C_{sat} (J K^{-1}mol^{-1})	265.3	268.7	272.4	276.7	281.7	287.7	294.7
Temp. (K)	660						
c_p (J K^{-1}g^{-1})	2.718						
C_p (J K^{-1}mol^{-1})	323.8						
c_{sat} (J K^{-1}g^{-1})	2.544						
C_{sat} (J K^{-1}mol^{-1})	303.1						

TABLE 62.60.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	31	31	0.618	1.11–1	0.33	9.40–3	1 0
Temp. range K	T_c K	A_1	A_2	A_3	A_4	A_5	A_6	Level of uncertainty
308.9–660.0	695.00	–2.56002	1.60328–1	9.90941	2.65753+1	–9.09894	1.09853	IV

Name: 2–Nitrobenzoic acid
Formula: $C_7H_5NO_4$

CAS–RN: 552–16–9
Group No.: 62–061
Molar Mass: 167.12

TABLE 62.61.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	419.0–513.0	eqn	nosp	not specified	C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.61.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.000	1.91–6	0.00	7.63–7	0
Temp. range K		A_1	A_2				Level of uncertainty
419.0–512.6		1.26735+1	5.03217				VI

TABLE 62.61.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	1.68	1.71	1.73	1.76	1.78	1.81	1.83
C_p (J K^{-1}mol^{-1})	281	285	289	294	298	302	306
Temp. (K)	490	500	510				
c_p (J K^{-1}g^{-1})	1.86	1.88	1.91				
C_p (J K^{-1}mol^{-1})	310	315	319				

Name: 3–Nitrobenzoic acid
Formula: $C_7H_5NO_4$

CAS–RN: 121–92–6
Group No.: 62–062
Molar Mass: 167.12

TABLE 62.62.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
26AND/LYN	N	415.0–498.0	eqn	nosp	not specified	C_p	DSIO	26AND/LYN

26AND/LYN calculated from temperature dependence of enthalpy by the compilers

TABLE 62.62.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.000	2.70–6	0.00	1.43–6	0
Temp. range K		A_1	A_2				Level of uncertainty
415.0–498.3		2.08823+1	4.83088				VI

TABLE 62.62.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	2.05	2.07	2.10	2.12	2.14	2.17	2.19
C_p (J K^{-1}mol^{-1})	342	346	350	354	358	362	366
Temp. (K)	490	500					
c_p (J K^{-1}g^{-1})	2.22	2.24					
C_p (J K^{-1}mol^{-1})	370	374					

Name: 4–Nitrobenzoic acid
Formula: $C_7H_5NO_4$

CAS–RN: 62–23–7
Group No.: 62–063
Molar Mass: 167.12

TABLE 62.63.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	512.3–518.2	2	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN constant value calculated from temperature dependence of enthalpy by the authors

TABLE 62.63.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
512.3–518.2	3.77412+1	VI

TABLE 62.63.4. Recommended values of heat capacities

Temp. (K)	515	520
c_p ($J\,K^{-1}g^{-1}$)	1.88	1.88
C_p ($J\,K^{-1}mol^{-1}$)	314	314

Name: 2–Methyl–1,3,5–trinitrobenzene
Formula: $C_7H_5N_3O_6$

CAS–RN: 118–96–7
Group No.: 62–064
Molar Mass: 227.13

TABLE 62.64.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
66ENI/PET	N	355.15	1.602	nosp	not specified		C_p	not specified	

66ENI/PET extrapolated from solid phase heat capacities obtained by Tomlinson W.R.Jr. etal., Picatinny Arsenal Techn. Rep. 1740(1958)319

Name: *N*–Methyl–*N*,2,4,6–tetranitrobenzeneamine
Formula: $C_7H_5N_5O_8$

CAS–RN: 479–45–8
Group No.: 62–065
Molar Mass: 287.15

TABLE 62.65.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KRI/LIC	N	419.50	1.445	nosp	not specified		C_{avg}	BDHT	73PER/COM

73KRI/LIC average value in temperature range 403–436 K

Name: 2–Methyl–1,3–dinitrobenzene
Formula: $C_7H_6N_2O_4$

CAS–RN: 606–20–2
Group No.: 62–066
Molar Mass: 182.14

TABLE 62.66.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
90FIN/PAY	N	335.0–365.0	13	nosp	99.93	melpt	C_p	BDHT	69PER/COM
90FIN/PAY	N	345.0–365.0	9	nosp	99.93	melpt	C_p	BDHT	69PER/COM

90FIN/PAY data for liquid form [A] with lower n.m.t.
90FIN/PAY data for liquid form [B] with higher n.m.t.

TABLE 62.66.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
90FIN/PAY	345.0–365.0	9	1.00#	0.238	7.63–2	0.24	3.65–4	–3
				Rejected data				
90FIN/PAY	(1.61, 4.79, 1.59, 9)							

TABLE 62.66.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	9	0.270	8.65–2	0.27	3.65–4	–3
Temp. range K		A_1	A_2				Level of uncertainty
345.0–365.0		1.30540+1	5.28192				IV

TABLE 62.66.4. Recommended values of heat capacities

Temp. (K)	350	360	370
c_p (J $K^{-1}g^{-1}$)	1.440	1.464	1.488
C_p (J $K^{-1}mol^{-1}$)	262.2	266.6	271.0

Name: Benzamide
Formula: C_7H_7NO

CAS–RN: 55–21–0
Group No.: 62–067
Molar Mass: 121.14

TABLE 62.67.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
35SKA	N	406.0–416.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN
90STE/CHI		415.0–475.0	4	nosp	99.95	chrom	C_p	BDHT	89KNI/ARC

35SKA temperature range not specified, recommended use near n.m.t.

TABLE 62.67.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
90STE/CHI	415.0–475.0	4	1.00#	0.290	9.80–2	0.29	5.56–4	0
				Rejected data				
35SKA	(2.11, 6.10, 2.11, 1)							

TABLE 62.67.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	4	0.411	1.39–1	0.41	5.56–4	0
Temp. range K		A_1	A_2				Level of uncertainty
415.0–475.0		1.93969+1	3.13918				IV

TABLE 62.67.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470	480
c_p (J K^{-1}g^{-1})	2.236	2.258	2.279	2.301	2.322	2.344	2.366
C_p (J K^{-1}mol^{-1})	270.9	273.5	276.1	278.7	281.3	283.9	286.6

Name: 1–Methyl–3–nitrobenzene
Formula: $C_7H_7NO_2$

CAS–RN: 99–08–1
Group No.: 62–068
Molar Mass: 137.14

TABLE 62.68.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
34KOL/UDO2	N	302.34	1.476	nosp	not specified		C_p	BSIT	34KOL/UDO2

34KOL/UDO2 same datum in 34KOL/UDO1

Name: 1–Methyl–4–nitrobenzene
Formula: $C_7H_7NO_2$

CAS–RN: 99–99–0
Group No.: 62–069
Molar Mass: 137.14

TABLE 62.69.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79RIC/SAV	315.0–340.0	eqn	1.10	99.9	estim	C_p	BDHT	69PER/COM

TABLE 62.69.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.000	1.48–6	0.00	2.72–7	0
Temp. range K		A_1	A_2				Level of uncertainty
315.0–340.2		1.59000+1	3.29877				IV

TABLE 62.69.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c_p ($J K^{-1} g^{-1}$)	1.604	1.624	1.644
C_p ($J K^{-1} mol^{-1}$)	220.0	222.7	225.5

Name: 1–Methoxy–2–nitrobenzene
Formula: $C_7H_7NO_3$

CAS–RN: 91–23–6
Group No.: 62–070
Molar Mass: 153.14

TABLE 62.70.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
59LUT/PAN	343.0–409.0	eqn	nosp	not specified		C_p	BDHO	58LUT/PAN
61ROU	298.4–310.9	5	nosp	not specified		C_p	BSAO	61ROU

TABLE 62.70.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
59LUT/PAN	343.0–408.7	10	3.00#	0.178	1.68–1	0.53	–6.11–2	2
61ROU	298.4–310.9	5	1.00#	0.341	1.04–1	0.34	1.47–2	3

TABLE 62.70.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.274	1.67–1	0.54	–3.58–2	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
298.4–408.7		4.62241+1	–1.16645+1	2.14843			V

TABLE 62.70.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350	360
c_p ($J K^{-1}g^{-1}$)	1.66	1.67	1.68	1.69	1.70	1.72	1.74
C_p ($J K^{-1}mol^{-1}$)	254	255	257	259	261	264	267
Temp. (K)	370	380	390	400	410		
c_p ($J K^{-1}g^{-1}$)	1.76	1.79	1.81	1.84	1.87		
C_p ($J K^{-1}mol^{-1}$)	270	274	278	282	287		

Name: 1–Methoxy–3–nitrobenzene
Formula: $C_7H_7NO_3$

CAS–RN: 555–03–3
Group No.: 62–071
Molar Mass: 153.14

TABLE 62.71.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59LUT/PAN	349.0–406.0	eqn	nosp	not specified		C_p	BDHO	58LUT/PAN

TABLE 62.71.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	1.91–6	0.00	–6.36–7	0
Temp. range K		A_1	A_2				Level of uncertainty
349.0–406.0		1.67743+1	4.26920				V

TABLE 62.71.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1}g^{-1}$)	1.72	1.75	1.77	1.79	1.81	1.84	1.86
C_p ($J K^{-1}mol^{-1}$)	264	267	271	274	278	281	285

Name: 1–Methoxy–4–nitrobenzene
Formula: $C_7H_7NO_3$

CAS–RN: 100–17–4
Group No.: 62–072
Molar Mass: 153.14

TABLE 62.72.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59LUT/PAN	348.0–408.0	eqn	nosp	not specified		C_p	BDHO	58LUT/PAN

TABLE 62.72.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.000	2.13–6	0.00	–9.54–7	0
Temp. range K		A_1	A_2				Level of uncertainty
348.0–408.0		1.31624+1	5.22476				V

TABLE 62.72.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390	400	410
c_p ($J K^{-1}g^{-1}$)	1.71	1.74	1.76	1.79	1.82	1.85	1.88
C_p ($J K^{-1}mol^{-1}$)	261	266	270	275	279	283	288

Name: Hexahydro–2(1*H*)–azocinone
Formula: $C_7H_{13}NO$

CAS–RN: 673–66–5
Group No.: 62–073
Molar Mass: 127.19

TABLE 62.73.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62KOL/PAU	N	315.0–350.0	7S	nosp	99.71	melpt	C_p	BSAO	56POP/KOL

62KOL/PAU some data in 59KOL/PAU

TABLE 62.73.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.011	1.71–3	0.01	1.09–6	0
Temp. range K		A_1	A_2				Level of uncertainty
315.0–350.0		5.27596	8.04187				IV

TABLE 62.73.4. Recommended values of heat capacities

Temp. (K)	320	330	340	350
c_p ($J K^{-1}g^{-1}$)	2.027	2.080	2.132	2.185
C_p ($J K^{-1}mol^{-1}$)	257.8	264.5	271.2	277.9

Name: *N*–Ethyl–*N*,2,4,6–tertranitrobenzeneamine
Formula: $C_8H_7N_5O_8$

CAS–RN: 6052–13–7
Group No.: 62–074
Molar Mass: 301.17

TABLE 62.74.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KRI/LIC	N	394.50	1.570	nosp	not specified		C_{avg}	BDHT	73PER/COM

73KRI/LIC average value in temperature range 369–420 K

Name: 3–Methyl–2,4,6–trinitro–*N*–(nitromethyl)benzenamine
Formula: $C_8H_7N_5O_8$

CAS–RN: 43072–20–4
Group No.: 62–075
Molar Mass: 301.17

TABLE 62.75.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73KRI/LIC	N	398.00	1.584	nosp	not specified		C_{avg}	BDHT	73PER/COM

73KRI/LIC average value in temperature range 376–420 K

Name: *N*–(2–Hydroxyphenyl)acetamide
Formula: $C_8H_9NO_2$

CAS–RN: 614–80–2
Group No.: 62–076
Molar Mass: 151.16

TABLE 62.76.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
26AND/LYN	N	365.0–413.0	eqn	nosp	not specified		C_p	DSIO	26AND/LYN

26AND/LYN unspecified isomer; probably *N*–(2–Hydroxyphenyl)acetamide (according to n.m.t.)

TABLE 62.76.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.000	2.95–6	0.00	–5.45–7	0

Temp. range K	A_1	A_2	Level of uncertainty
365.0–413.0	1.35476+1	6.03861	VI

TABLE 62.76.4. *Recommended values of heat capacities*

Temp. (K)	370	380	390	400	410
c_p ($J\,K^{-1}g^{-1}$)	1.97	2.01	2.04	2.07	2.11
C_p ($J\,K^{-1}mol^{-1}$)	298	303	308	313	318

Name: Methyl ester phenylcarbamic acid
Formula: $C_8H_9NO_2$

CAS–RN: 2603–10–3
Group No.: 62–077
Molar Mass: 151.16

TABLE 62.77.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71PRI	335.0–390.0	eqn	3.00	not specified		C_p	BDHT	65GOD/BAR

TABLE 62.77.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
335.0–390.0		1.76479+1	4.79233				VI

TABLE 62.77.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390
c_p ($J K^{-1}g^{-1}$)	1.87	1.89	1.92	1.95	1.97	2.00
C_p ($J K^{-1}mol^{-1}$)	282	286	290	294	298	302

Name: 1,6–Diisocyanatohexane
Formula: $C_8H_{12}N_2O_2$

CAS–RN: 822–06–0
Group No.: 62–078
Molar Mass: 168.20

TABLE 62.78.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
62STR/BAR	N	310.6	1	1.00	99.9	anal	C_{avg}	DSIO	62STR/BAR
85LEB/BYK2		206.1–330.0	4S	0.30	99.53	melpt	C_p	BSAO	76LEB/LIT

62STR/BAR average value in temperature range 298–323 K

TABLE 62.78.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
62STR/BAR	310.6	1	1.00	0.588	2.12–1	0.59	2.12–1	1
85LEB/BYK2	206.1–330.0	4	0.30	0.817	8.35–2	0.25	–4.21–3	0

TABLE 62.78.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	1.003	1.56–1	0.44	3.90–2	1
Temp. range K		A_1	A_2				Level of uncertainty
206.1–330.0		2.68283+1	2.87511				IV

TABLE 62.78.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.625	1.639	1.653	1.667	1.682	1.696	1.710
C_p (J K^{-1}mol^{-1})	273.3	275.7	278.0	280.4	282.8	285.2	287.6
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.714	1.724	1.738	1.750	1.753	1.767	1.781
C_p (J K^{-1}mol^{-1})	288.4	290.0	292.4	294.3	294.8	297.2	299.6
Temp. (K)	330						
c_p (J K^{-1}g^{-1})	1.795						
C_p (J K^{-1}mol^{-1})	302.0						

Name: *N*,*N*–Dipropylacetamide
Formula: $C_8H_{17}NO$

CAS–RN: 1116–24–1
Group No.: 62–079
Molar Mass: 143.23

TABLE 62.79.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
84ZEG/SOM1	298.15	2.094	0.30	99.5	chrom	C_p	FSIT	71PIC/LED

Name: Bis(1,1–dimethylethyl)diazene 1–oxide
Formula: $C_8H_{18}N_2O$

CAS–RN: 16649–52–8
Group No.: 62–080
Molar Mass: 158.24

TABLE 62.80.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81BYS	298.15	2.000	nosp	99.9	melpt	C_p	BDHT	69PER/COM

Name: 2,4–Diisocyanato–1–methylbenzene
Formula: $C_9H_6N_2O_2$

CAS–RN: 584–84–9
Group No.: 62–081
Molar Mass: 174.16

TABLE 62.81.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
62STR/BAR	N	310.6	1	1.00	99.9	anal	C_{avg}	DSIO	62STR/BAR
72STR/NOV	N	300.1–313.1	2	nosp	98.	estim	C_p	DSIO	62STR/BAR

62STR/BAR average value in temperature range 298–323 K
72STR/NOV technical product, purity in question

TABLE 62.81.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
72STR/NOV	300.1–313.1	2	5.00#	0.000	0.00	0.00	0.00	0
				Rejected data				
62STR/BAR	(1.53+1, 44.14, 1.53+1, 1)							

TABLE 62.81.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
300.1–313.1		4.67829	4.71906				VI

TABLE 62.81.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p ($J K^{-1} g^{-1}$)	0.90	0.92
C_p ($J K^{-1} mol^{-1}$)	157	161

Name: Ethyl ester phenylcarbamic acid
Formula: $C_9H_{11}NO_2$

CAS–RN: 101–99–5
Group No.: 62–082
Molar Mass: 165.19

TABLE 62.82.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71PRI	340.0–390.0	eqn	3.00	not specified		C_p	BDHT	65GOD/BAR

TABLE 62.82.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.000	2.20–6	0.00	–7.63–7	0
Temp. range K		A_1	A_2				Level of uncertainty
340.0–390.0		1.61267+1	6.56706				VI

TABLE 62.82.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390
c_p (J K^{-1}g^{-1})	1.94	1.97	2.00	2.03	2.07	2.10
C_p (J K^{-1}mol^{-1})	320	325	331	336	342	347

Name: Tetraethyl urea
Formula: $C_9H_{20}N_2O$

CAS–RN: 1187–03–7
Group No.: 62–083
Molar Mass: 172.27

TABLE 62.83.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
90KOZ/SIM	290.0–370.0	eqn	2.00	not specified		C_p	BDHT	92KAB/KOZ

TABLE 62.83.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.000	3.12–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
290.0–369.8		2.83540+1	4.83372				V

TABLE 62.83.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_p (J K^{-1}g^{-1})	2.05	2.06	2.07	2.09	2.12	2.14	2.16
C_p (J K^{-1}mol^{-1})	352	356	356	360	364	368	372
Temp. (K)	350	360	370				
c_p (J K^{-1}g^{-1})	2.19	2.21	2.23				
C_p (J K^{-1}mol^{-1})	376	380	384				

Name: 1–Nitronaphthalene
Formula: $C_{10}H_7NO_2$

CAS–RN: 86–57–7
Group No.: 62–084
Molar Mass: 173.17

TABLE 62.84.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
*84BAT	N	360.6	1	nosp	not specified		C_p	not specified	
*95SCH		367.5	1	0.50	not specified		C_{avg}	not specified	
13CAM	N	331.8–334.5	2	nosp	not specified		C_p	not specified	

*84BAT error 0.5 % (information in 29WAS)
13CAM error 0.5 % (information in 29WAS)

TABLE 62.84.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
*95SCH	367.5	1	0.50	0.028	4.83–3	0.01	–4.83–3	–1
13CAM	331.8–334.5	2	1.50#	0.998	4.86–1	1.50	3.62–2	0
				Rejected data				
*84BAT	(1.41, 4.01, 1.41, 1)							

TABLE 62.84.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	3	1.412	6.87–1	2.12	2.25–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
331.8–367.5		1.62636+1	4.82565				V

TABLE 62.84.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	1.57	1.59	1.61	1.64
C_p ($J\,K^{-1}mol^{-1}$)	272	276	280	284

Name: Propyl ester phenylcarbamic acid
Formula: $C_{10}H_{13}NO_2$

CAS–RN: 5532–90–1
Group No.: 62–085
Molar Mass: 179.22

TABLE 62.85.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71PRI	340.0–400.0	eqn	3.00	not specified		C_p	BDHT	65GOD/BAR

TABLE 62.85.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	2.70–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
340.0–400.0		1.98409+1	7.57561				VI

TABLE 62.85.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	2.12	2.15	2.19	2.22	2.26	2.29	2.33
C_p (J K^{-1}mol^{-1})	379	385	392	398	404	411	417

Name: *E*–(*R*,*S*)–2–Methyl–5–(1–methylethenyl)–2–cyclohexen–1–one oxime
Formula: $C_{10}H_{15}NO$

CAS–RN: 55658–55–4
Group No.: 62–086
Molar Mass: 165.24

TABLE 62.86.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77MEI/BLO	366.4–386.8	9	nosp	99.6	melpt	C_{sat}	BSAO	72VAN

TABLE 62.86.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	9	9	0.181	4.09–2	0.09	5.68–5	0
Temp. range K		A_1	A_2				Level of uncertainty
366.4–386.8		1.77380+1	7.31247				III

TABLE 62.86.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_{sat} (J K^{-1}g^{-1})	2.254	2.291	2.328
C_{sat} (J K^{-1}mol^{-1})	372.4	378.5	384.6

Name: [*R*–(*E*)]–2–Methyl–5–(1–methylethenyl)–2–cyclohexen–1–one oxime
Formula: $C_{10}H_{15}NO$

CAS–RN: 60827–56–7
Group No.: 62–087
Molar Mass: 165.24

TABLE 62.87.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
77MEI/BLO	348.6–384.8	10	nosp	99.6	melpt	C_{sat}	BSAO	72VAN

TABLE 62.87.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.196	4.43–2	0.10	6.48–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
348.6–384.8	1.50282+1	8.14196	III

TABLE 62.87.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380
c_{sat} (J K^{-1}g^{-1})	2.190	2.231	2.272	2.313
C_{sat} (J K^{-1}mol^{-1})	361.9	368.7	375.4	382.2

Name: *N*,*N*–Dibutylacetamide
Formula: $C_{10}H_{21}NO$

CAS–RN: 1563–90–2
Group No.: 62–088
Molar Mass: 171.28

TABLE 62.88.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84ZEG/SOM1	298.15	2.103	0.30	99.5	chrom	C_p	FSIT	71PIC/LED

Name: 1,1'–Oxybis(4–nitrobenzene)
Formula: $C_{12}H_8N_2O_5$

CAS–RN: 101–63–3
Group No.: 62–089
Molar Mass: 260.21

TABLE 62.89.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78MAR/CIO1	N	420.0–490.0	8S	nosp	not specified		C_p	DSIO	71MAR/CIO

78MAR/CIO1 values calculated from temperature dependence of enthalpy by the authors; suspect values

Name: 4,4'–Oxybisbenzenamine
Formula: $C_{12}H_{12}N_2O$

CAS–RN: 101–80–4
Group No.: 62–090
Molar Mass: 200.24

TABLE 62.90.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78MAR/CIO1	N	470.0–500.0	4S	nosp	not specified		C_p	DSIO	71MAR/CIO
87LES/LIC	N	455.0–500.0	eqn	2.00	99.	estim	C_p	BDHT	69PER/COM

78MAR/CIO1 values calculated from temperature dependence of enthalpy by the authors; suspect values
87LES/LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 62.90.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
87LES/LIC	455.0–500.0	11	2.00	0.000	1.99–6	0.00	3.47–7	0
				Rejected data				
78MAR/CIO1	(3.69+3, 98.54, 3.69+3, 4)							

TABLE 62.90.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	11	0.000	2.20–6	0.00	3.47–7	0
Temp. range K		A_1	A_2				Level of uncertainty
455.0–500.0		2.69644+1	5.73703				V

TABLE 62.90.4. Recommended values of heat capacities

Temp. (K)	460	470	480	490	500
c_p ($J K^{-1} g^{-1}$)	2.22	2.24	2.26	2.29	2.31
C_p ($J K^{-1} mol^{-1}$)	444	448	453	458	463

Name: *N*,*N*'–Dipropylhexanediamine
Formula: $C_{12}H_{24}N_2O_2$

CAS–RN: 10263–96–4
Group No.: 62–091
Molar Mass: 228.33

TABLE 62.91.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53WIL/DOL	463.1–483.1	3S	nosp	not specified		C_p	BSAO	51DOL/HET

TABLE 62.91.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.812	6.10–1	0.81	3.28–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
463.1–483.1		3.38319+1	8.67432				IV

TABLE 62.91.4. Recommended values of heat capacities

Temp. (K)	460	470	480
c_p (J $K^{-1}g^{-1}$)	2.685	2.717	2.748
C_p (J $K^{-1}mol^{-1}$)	613.1	620.3	627.5

Name: *N*,*N*–Dipentylacetamide
Formula: $C_{12}H_{25}NO$

CAS–RN: 16238–16–7
Group No.: 62–092
Molar Mass: 199.34

TABLE 62.92.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
84ZEG/SOM1	298.15	2.098	0.30	99.5	chrom	C_p	FSIT	71PIC/LED

Name: 1–(1–Isocyanato–1–methylethyl)–3–(1–methylethenyl)benzene
Formula: $C_{13}H_{15}NO$

CAS–RN: 2094–99–7
Group No.: 62–093
Molar Mass: 201.27

TABLE 62.93.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86ACH/HAS	333.1–433.1	2	3.00	98.	chrom	C_p	BDHT	69PER/COM

TABLE 62.93.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
333.1–433.1		2.98640+1	4.84137				VI

TABLE 62.93.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p (J K^{-1}g^{-1})	1.89	1.91	1.93	1.95	1.97	1.99	2.01
C_p (J K^{-1}mol^{-1})	381	385	389	393	397	401	405
Temp. (K)	400	410	420	430			
c_p (J K^{-1}g^{-1})	2.03	2.05	2.07	2.09			
C_p (J K^{-1}mol^{-1})	409	413	417	421			

Name: 1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene
Formula: $C_{13}H_{15}NO$

CAS-RN: 2889-58-9
Group No.: 62-094
Molar Mass: 201.27

TABLE 62.94.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
86ACH/HAS	333.1-433.1	2	3.00	91.	chrom	C_p	BDHT	69PER/COM

TABLE 62.94.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
333.1-433.1		3.55078+1	2.42069				VI

TABLE 62.94.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p (J K^{-1}g^{-1})	1.80	1.81	1.82	1.83	1.84	1.85	1.86
C_p (J K^{-1}mol^{-1})	362	364	366	368	370	372	374
Temp. (K)	400	410	420	430			
c_p (J K^{-1}g^{-1})	1.87	1.88	1.89	1.90			
C_p (J K^{-1}mol^{-1})	376	378	380	382			

Name: Hexyl ester phenylcarbamic acid
Formula: $C_{13}H_{19}NO_2$

CAS-RN: 7461-26-9
Group No.: 62-095
Molar Mass: 221.30

TABLE 62.95.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71PRI	340.0-400.0	eqn	3.00	not specified		C_p	BDHT	65GOD/BAR

TABLE 62.95.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	2.70–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
340.0–400.0		4.26515+1	5.12262				VI

TABLE 62.95.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1}g^{-1}$)	2.26	2.28	2.30	2.31	2.33	2.35	2.37
C_p ($J K^{-1}mol^{-1}$)	499	504	508	512	516	521	525

Name: Bis(4–methoxyphenyl)diazene–1–oxide
Formula: $C_{14}H_{14}N_2O_3$

CAS–RN: 1562–94–3
Group No.: 62–096
Molar Mass: 258.28

TABLE 62.96.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38KRE	411.0	1	2.00	not specified		C_p	BDHT	38KRE
64ARN2	408.2–423.1	11S	0.30	not specified		C_p	BSAO	64ARN1
67BAR/POR	410.1–423.1	8S	3.00	99.9	anal	C_p	BDHT	73PER/COM

TABLE 62.96.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	408.6–423.1	10	0.80#	1.010	5.07–1	0.81	8.57–3	2
				Rejected data				
38KRE	(1.06, 1.68, 1.06, 1)			67BAR/POR	(7.59–1, 1.25,–5.55–1, –6)			

TABLE 62.96.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	10	1.207	6.06–1	0.97	8.57–3	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
408.6–423.1		5.45467+3	–2.57973+3	3.08448+2			IV

TABLE 62.96.4. Recommended values of heat capacities

Temp. (K)	410	420
c_p ($J K^{-1} g^{-1}$)	2.022	1.959
C_p ($J K^{-1} mol^{-1}$)	522.3	506.0

Name: 1,3–Bis(1–isocyanato–1–methylethyl)benzene
Formula: $C_{14}H_{16}N_2O_2$

CAS–RN: 2778–42–9
Group No.: 62–097
Molar Mass: 244.29

TABLE 62.97.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86ACH/HAS	333.1–433.1	2	3.00	99.	chrom	C_p	BDHT	69PER/COM

TABLE 62.97.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
333.1–433.1		4.60365+1	2.93816				VI

TABLE 62.97.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	1.90	1.91	1.92	1.93	1.94	1.95	1.96
C_p ($J K^{-1} mol^{-1}$)	463	466	468	471	473	476	478
Temp. (K)	400	410	420	430			
c_p ($J K^{-1} g^{-1}$)	1.97	1.98	1.99	2.00			
C_p ($J K^{-1} mol^{-1}$)	480	483	485	488			

Name: 1,4–Bis(1–isocyanato–1–methylethyl)benzene
Formula: $C_{14}H_{16}N_2O_2$

CAS–RN: 2778–41–8
Group No.: 62–098
Molar Mass: 244.29

TABLE 62.98.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86ACH/HAS	433.15	1.900	3.00	99.	chrom	C_p	BDHT	69PER/COM

Name: 1,1'–Methylenebis[4–isocyanatobenzene]
Formula: $C_{15}H_{10}N_2O_2$

CAS–RN: 101–68–8
Group No.: 62–099
Molar Mass: 250.26

TABLE 62.99.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
66ZAL/STR	N	335.1	1	nosp	not specified		C_{avg}	not specified	
77LEB/EVS3		321.3–331.5	9	0.30	99.81	melpt	C_p	BSAO	66NIK/LEB

66ZAL/STR average value in temperature range 319–351 K

TABLE 62.99.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
77LEB/EVS3	321.3–331.5	9	0.30	0.160	2.27–2	0.05	1.95–5	2

TABLE 62.99.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	9	0.181	2.58–2	0.05	1.95–5	2
Temp. range K		A_1	A_2				Level of uncertainty
321.3–331.5		3.26835+1	4.52970				III

TABLE 62.99.4. Recommended values of heat capacities

Temp. (K)	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.567	1.583
C_p ($J\,K^{-1}mol^{-1}$)	392.3	396.0

Name: (4–Ethoxyphenyl)(4–methoxyphenyl)diazene–*N*–oxide
Formula: $C_{15}H_{16}N_2O_3$

CAS–RN: 56095–14–8
Group No.: 62–100
Molar Mass: 272.30

TABLE 62.100.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
38KRE	429.65	1.757	2.00	not specified		C_p	BDHT	38KRE

Name: [(4–Methoxyphenyl)methylene]hydrazone–4–methoxybenzaldehyde
Formula: $C_{16}H_{16}N_2O_2$

CAS–RN: 2299–73–2
Group No.: 62–101
Molar Mass: 268.32

TABLE 62.101.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67BAR/POR	N	473.1–510.1	5	nosp	99.9	anal	C_p	BDHT	73PER/COM

67BAR/POR data from a graph only

TABLE 62.101.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.662	4.95–1	0.66	4.05–3	1

Temp. range K	A_1	A_2	Level of uncertainty
473.1–510.1	1.29084+1	1.23556+1	V

TABLE 62.101.4. Recommended values of heat capacities

Temp. (K)	470	480	490	500	510
c_p ($J K^{-1} g^{-1}$)	2.20	2.24	2.28	2.31	2.35
C_p ($J K^{-1} mol^{-1}$)	590	600	611	621	631

Name: Bis(4–ethoxyphenyl)diazene–1–oxide
Formula: $C_{16}H_{18}N_2O_3$

CAS–RN: 4792–83–0
Group No.: 62–102
Molar Mass: 286.33

TABLE 62.102.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
38KRE	438.1	1	2.00	not specified		C_p	BDHT	38KRE
64ARN2	440.5–453.1	9S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	454.0–459.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.102.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	441.1–453.1	8	0.80#	0.654	4.05–1	0.52	1.90–4	0
64ARN2	454.0–459.0	3	0.80#	0.432	2.61–1	0.35	1.14–2	1

TABLE 62.102.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	11	0.705	4.35–1	0.56	3.24–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
441.1–459.0		4.95837+3	–2.15941+3	2.38724+2			IV

TABLE 62.102.4. Recommended values of heat capacities

Temp. (K)	440	450	460
c_p (J K^{-1}g^{-1})	2.284	2.183	2.221
C_p (J K^{-1}mol^{-1})	654.1	625.2	636.0

Name: Nonyl phenylcarbamate
Formula: $C_{16}H_{25}NO_2$

CAS–RN: 33689–71–3
Group No.: 62–103
Molar Mass: 263.38

TABLE 62.103.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71PRI	340.0–395.0	eqn	3.00	not specified		C_p	BDHT	65GOD/BAR

TABLE 62.103.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.000	5.39–6	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
340.0–395.0		2.91581+1	1.28561+1				VI

TABLE 62.103.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p (J K^{-1}g^{-1})	2.30	2.34	2.38	2.42	2.46	2.50	2.54
C_p (J K^{-1}mol^{-1})	606	617	627	638	649	659	670

Name: Diethyl ester 4,4'–azoxybisbenzoic acid
Formula: $C_{18}H_{18}N_2O_5$

CAS–RN: 6421–04–1
Group No.: 62–104
Molar Mass: 342.35

TABLE 62.104.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
32SPA/THO	403.1–423.1	3S	1.00	not specified		C_p	BDHO	31THO/PAR

TABLE 62.104.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	Level of uncertainty
403.1–423.1	6.04787+1	5.16830	IV

TABLE 62.104.4. Recommended values of heat capacities

Temp. (K)	400	410	420
c_p ($J\,K^{-1}g^{-1}$)	1.971	1.983	1.996
C_p ($J\,K^{-1}mol^{-1}$)	674.7	679.0	683.3

Name: 4–Butyl–*N*–[(4–methoxyphenyl)methylene]benzenamine
Formula: $C_{18}H_{21}NO$

CAS–RN: 26227–73–6
Group No.: 62–105
Molar Mass: 267.37

TABLE 62.105.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74SHI/MAE	320.7–330.0	12	nosp	99.976	melpt	C_p	BSAO	73SHI/ENO

TABLE 62.105.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.807	1.95–1	0.32	–2.65–2	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
320.7–330.0	4.64255+5	–4.25391+5	1.29936+5	–1.32289+4	III

TABLE 62.105.4. Recommended values of heat capacities

Temp. (K)	320	325	330
c_p ($J\,K^{-1}g^{-1}$)	1.939	1.816	1.843
C_p ($J\,K^{-1}mol^{-1}$)	518.4	485.5	492.7

Name: 2–[[(4–Butylphenyl)imino]methyl]–4–methoxyphenol
Formula: $C_{18}H_{21}NO_2$

CAS–RN: 52218–22–1
Group No.: 62–106
Molar Mass: 283.37

TABLE 62.106.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73SOR/SEK	334.7–371.8	14	nosp	99.393	melpt	C_{sat}	BSAO	65SUG/SEK

TABLE 62.106.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	14	1.356	3.56–1	0.54	3.00–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
334.7–371.8		3.59718+2	–1.72021+2	2.50809+1			IV

TABLE 62.106.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_{sat} (J K^{-1}g^{-1})	1.901	1.904	1.922	1.954
C_{sat} (J K^{-1}mol^{-1})	538.6	539.5	544.5	553.7

Name: (*E*)–(4–Butylphenyl)(4–ethoxyphenyl)diazene
Formula: $C_{18}H_{22}N_2O$

CAS–RN: 98644–12–3
Group No.: 62–107
Molar Mass: 282.39

TABLE 62.107.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85SHA/ZHU	357.1–362.8	7	0.50	not specified		C_p	BSAO	87KHO/BUG

TABLE 62.107.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.397	1.37–1	0.20	2.74–4	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
357.1–362.8		6.02472+3	–3.29093+3	4.54564+2			IV

TABLE 62.107.4. Recommended values of heat capacities

Temp. (K)	360
c_p (J K^{-1}g^{-1})	2.017
C_p (J K^{-1}mol^{-1})	569.6

Name: Bis(4–propoxyphenyl)diazene–1–oxide
Formula: $C_{18}H_{22}N_2O_3$

CAS–RN: 23315–55–1
Group No.: 62–108
Molar Mass; 314.38

TABLE 62.108.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
64ARN2	396.6–413.1	9S	0.30	not specified	C_p	BSAO	64ARN1
64ARN2	422.0–447.0	eqn	0.30	not specified	C_p	BSAO	64ARN1

TABLE 62.108.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	397.6–413.1	7	0.80#	0.780	5.06–1	0.62	–5.71–2	–3
64ARN2	422.0–447.2	8	0.80#	0.289	1.88–1	0.23	5.62–2	3

TABLE 62.108.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	17	15	0.641	4.16–1	0.51	3.37–3	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
397.6–447.2		5.05017+2	–2.04215+2	2.45264+1			IV

TABLE 62.108.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	2.131	2.116	2.115	2.126	2.150	2.187
C_p ($J K^{-1} mol^{-1}$)	670.0	665.4	664.8	668.4	676.0	687.7

Name: *N*,*N*'–Dihexylhexanediamide
Formula: $C_{18}H_{36}N_2O_2$

CAS–RN: 21150–82–3
Group No.: 62–109
Molar Mass: 312.50

TABLE 62.109.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
53WIL/DOL	443.1–483.1	5S	nosp	not specified	C_p	BSAO	51DOL/HET

TABLE 62.109.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.955	7.72–1	0.76	4.78–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
443.1–483.1		9.36613+2	–3.56322+2	3.79626+1			IV

TABLE 62.109.4. Recommended values of heat capacities

Temp. (K)	440	450	460	470	480
c_p (J $K^{-1}g^{-1}$)	2.760	2.711	2.682	2.674	2.685
C_p (J $K^{-1}mol^{-1}$)	862.6	847.3	838.2	835.5	839.1

Name: 4–Butyl–*N*–[(4–ethoxyphenyl)methylene]benzenamine
Formula: $C_{19}H_{23}NO$

CAS–RN: 29743–08–6
Group No.: 62–110
Molar Mass: 281.40

TABLE 62.110.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74SOR/NAK	349.5–371.7	14	nosp	99.75	melpt	C_p	BSAO	65SUG/SEK

TABLE 62.110.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	1.669	6.03–1	0.83	7.85–3	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
349.5–371.7		1.91729+3	–1.01946+3	1.40654+2			IV

TABLE 62.110.4. Recommended values of heat capacities

Temp. (K)	350	360	370
c_p (J $K^{-1}g^{-1}$)	2.133	2.072	2.093
C_p (J $K^{-1}mol^{-1}$)	600.3	583.0	589.1

Name: *N*–[[4–(Hexyloxy)phenyl]methylene]benzenamine
Formula: $C_{19}H_{23}NO$

CAS–RN: 5219–49–8
Group No.: 62–111
Molar Mass: 281.40

TABLE 62.111.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TSU/SOR3	323.8–386.7	15	nosp	99.86	melpt	C_p	BSAO	83YOS/SOR1

TABLE 62.111.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.368	7.71–2	0.11	1.77–4	–3
Temp. range K		A_1	A_2				Level of uncertainty
323.8–386.7		3.84488+1	8.49018				III

TABLE 62.111.4. Recommended values of heat capacities

Temp. (K)	330	340	350	360	370	380	390
c_p ($J\,K^{-1}g^{-1}$)	1.964	1.989	2.014	2.039	2.064	2.089	2.114
C_p ($J\,K^{-1}mol^{-1}$)	552.6	559.7	566.8	573.8	580.9	587.9	595.0

Name: 4–[[[4–(Hexyloxy)phenyl]methylene]amino]benzonitrile
Formula: $C_{20}H_{22}N_2O$

CAS–RN: 35280–78–5
Group No.: 62–112
Molar Mass: 306.41

TABLE 62.112.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79TSU/SOR	377.5–385.3	4	0.20	99.9	melpt	C_p	BSAO	83YOS/SOR1

TABLE 62.112.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.775	1.20–1	0.15	–9.54–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
377.5–385.3		6.91752+3	–3.55227+3	4.61142+2			II

TABLE 62.112.4. Recommended values of heat capacities

Temp. (K)	380	390
c_p ($J K^{-1} g^{-1}$)	2.111	2.107
C_p ($J K^{-1} mol^{-1}$)	646.8	645.6

Name: (*E*)–4–[(4–Methoxyphenyl)azo]phenyl ester heptanoic acid
Formula: $C_{20}H_{24}N_2O_3$

CAS–RN: 97402–83–0
Group No.: 62–113
Molar Mass: 340.42

TABLE 62.113.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85SHA/ZHU	372.5–373.9	4	0.50	not specified		C_p	BSAO	87KHO/BUG

TABLE 62.113.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.514	2.21–1	0.26	5.40–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
372.5–373.9		6.38680+2	–1.48013+2				IV

TABLE 62.113.4. Recommended values of heat capacities

Temp. (K)	372	374
c_p ($J K^{-1} g^{-1}$)	2.151	2.079
C_p ($J K^{-1} mol^{-1}$)	732.3	707.7

Name: *N*–[[4–(Hexyloxy)phenyl]methylene]–4–methylbenzenamine
Formula: $C_{20}H_{25}NO$

CAS–RN: 25959–51–7
Group No.: 62–114
Molar Mass: 295.42

TABLE 62.114.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82TSU/SOR4	347.6–385.3	14	nosp	99.84	melpt	C_p	BSAO	83YOS/SOR1

TABLE 62.114.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	2.377	5.49–1	0.71	6.00–3	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
348.4–385.3		8.14634+2	–4.01534+2	5.44944+1			III

TABLE 62.114.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390
c_p (J K^{-1}g^{-1})	2.162	2.121	2.110	2.131	2.182
C_p (J K^{-1}mol^{-1})	638.7	626.6	623.5	629.4	644.5

Name: Bis(4–butoxyphenyl)diazene–1–oxide
Formula: $C_{20}H_{26}N_2O_3$

CAS–RN: 17051–01–3
Group No.: 62–115
Molar Mass: 342.44

TABLE 62.115.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
64ARN2	409.8–428.1	9S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	429.0–448.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.115.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	410.1–428.1	8	0.70#	2.090	1.41	1.46	–1.11–1	–2
64ARN2	429.0–448.0	6	0.70#	0.932	5.95–1	0.65	2.11–1	2

TABLE 62.115.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	14	1.911	1.28	1.34	2.69–2	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
410.1–448.0		1.98512+3	–8.76494+2	1.01353+2			IV

TABLE 62.115.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440	450
c_p (J K^{-1}g^{-1})	2.312	2.227	2.190	2.203	2.265
C_p (J K^{-1}mol^{-1})	791.9	762.5	750.1	754.5	775.7

Name: 1,1'–(Methylenedi–4,1–phenylene)bis–1*H*–pyrrole–2,5–dione
Formula: $C_{21}H_{14}N_2O_4$

CAS–RN: 13676–54–5
Group No.: 62–116
Molar Mass: 358.35

TABLE 62.116.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78MAR/CIO1	N	430.0–570.0	15S	nosp	not specified		C_p	DSIO	71MAR/CIO

78MAR/CIO1 values calculated from temperature dependence of enthalpy by the authors; suspect values

Name: 4–Butyl–*N*–[[4–(pentyloxy)phenyl]methylene]benzenamine
Formula: $C_{22}H_{29}NO$

CAS–RN: 29743–10–0
Group No.: 62–117
Molar Mass: 323.48

TABLE 62.117.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83SOR/TAN	342.7–389.8	19	nosp	99.92	melpt	C_p	BSAO	83YOS/SOR1

TABLE 62.117.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	17	1.858	4.69–1	0.56	4.31–3	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
344.2–389.8		5.00885+2	–2.29989+2	3.16143+1			III

TABLE 62.117.4. Recommended values of heat capacities

Temp. (K)	350	360	370	380	390
c_p ($J\,K^{-1}g^{-1}$)	2.138	2.124	2.126	2.145	2.179
C_p ($J\,K^{-1}mol^{-1}$)	691.8	687.2	687.8	693.7	704.9

Name: Bis(4–pentyloxyphenyl)diazene–1–oxide
Formula: $C_{22}H_{30}N_2O_3$

CAS–RN: 19482–05–4
Group No.: 62–118
Molar Mass: 370.49

TABLE 62.118.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64ARN2	396.3–423.1	10S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	424.0–444.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.118.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	398.1–423.1	8	0.70#	0.732	5.20–1	0.51	–6.57–2	0
64ARN2	424.0–444.0	5	0.70#	0.472	3.31–1	0.33	1.16–1	3

TABLE 62.118.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	13	0.735	5.21–1	0.51	4.12–3	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
398.1–444.0		7.84101+2	–3.24113+2	3.83554+1			IV

TABLE 62.118.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440
c_p (J K^{-1}g^{-1})	2.274	2.244	2.231	2.235	2.257
C_p (J K^{-1}mol^{-1})	842.6	831.4	826.6	828.2	836.1

Name: *N*,*N*'–Dihexyldecanediamine
Formula: $C_{22}H_{44}N_2O_2$

CAS–RN: 31827–03–9
Group No.: 62–119
Molar Mass: 368.60

TABLE 62.119.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
53WIL/DOL	423.1–483.1	7S	nosp	not specified		C_p	BSAO	51DOL/HET

TABLE 62.119.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	6	0.070	6.77–2	0.06	5.47–5	1
Temp. range K		A_1	A_2				Level of uncertainty
433.1–483.1		7.38706+1	1.03813+1				IV

TABLE 62.119.4. Recommended values of heat capacities

Temp. (K)	430	440	450	460	470	480
c_p ($J K^{-1} g^{-1}$)	2.673	2.697	2.720	2.743	2.767	2.790
C_p ($J K^{-1} mol^{-1}$)	985.4	994.0	1003	1011	1020	1029

Name: 4–Butyl–*N*–[[4–(hexyloxy)phenyl]methylene]benzenamine
Formula: $C_{23}H_{31}NO$

CAS–RN: 29743–11–1
Group No.: 62–120
Molar Mass: 337.51

TABLE 62.120.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83YOS/SOR2	351.5–390.6	16	nosp	99.93	melpt	C_p	BSAO	83YOS/SOR1

TABLE 62.120.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	15	2.883	7.95–1	0.86	1.10–2	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
352.1–390.6	1.21577+3	–6.01857+2	8.03130+1	IV

TABLE 62.120.4. Recommended values of heat capacities

Temp. (K)	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	2.216	2.177	2.179	2.219
C_p ($J K^{-1} mol^{-1}$)	747.8	734.9	735.3	749.1

Name: Bis(4–hexyloxyphenyl)diazene–1–oxide
Formula: $C_{24}H_{34}N_2O_3$

CAS–RN: 2587–42–0
Group No.: 62–121
Molar Mass: 398.55

TABLE 62.121.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64ARN2	402.2–428.1	9S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	432.0–448.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.121.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
64ARN2	403.1–428.1	8	0.70#	1.741	1.41	1.22	–5.25–2	0
64ARN2	432.0–448.0	5	0.70#	0.809	6.26–1	0.57	1.46–1	1

TABLE 62.121.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	14	13	1.659	1.34	1.16	2.40–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
403.1–448.0		1.60474+3	–6.93140+2	8.03339+1			IV

TABLE 62.121.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	2.363	2.308	2.287	2.299	2.344
C_p ($J K^{-1} mol^{-1}$)	941.9	919.9	911.4	916.2	934.3

Name: Bis(4–heptyloxyphenyl)diazene–1–oxide
Formula: $C_{26}H_{38}N_2O_3$

CAS–RN: 2635–26–9
Group No.: 62–122
Molar Mass: 426.60

TABLE 62.122.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
64ARN2	397.4–433.1	12S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	434.0–447.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.122.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
64ARN2	399.1–433.1	10	0.70#	1.121	9.81–1	0.78	1.93–2	0
64ARN2	434.0–447.2	5	0.70#	0.609	5.12–1	0.43	–2.66–3	1

TABLE 62.123.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	18	16	1.268	1.20	0.89	1.77–2	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
401.1–452.2		1.87718+3	–8.06307+2	9.28907+1			IV

TABLE 62.123.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450
c_p (J $K^{-1}g^{-1}$)	2.527	2.429	2.364	2.334	2.337	2.374
C_p (J $K^{-1}mol^{-1}$)	1149	1104	1075	1061	1063	1080

Name: Bis(4–nonyloxyphenyl)diazene–1–oxide
Formula: $C_{30}H_{46}N_2O_3$

CAS–RN: 25729–13–9
Group No.: 62–124
Molar Mass: 482.71

TABLE 62.124.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
64ARN2	394.4–433.1	13S	0.30	not specified	C_p	BSAO	64ARN1
64ARN2	435.0–447.0	eqn	0.30	not specified	C_p	BSAO	64ARN1

TABLE 62.124.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
64ARN2	397.1–433.1	10	0.70#	1.097	1.12	0.77	3.52–2	0
64ARN2	435.0–447.0	5	0.70#	0.726	6.98–1	0.51	–2.78–2	1

TABLE 62.124.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	18	15	1.106	1.12	0.77	1.42–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
397.1–447.0		2.11947+3	–9.19281+2	1.06518+2			IV

TABLE 62.124.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450
c_p (J K^{-1}g^{-1})	2.526	2.428	2.368	2.344	2.357	2.406
C_p (J K^{-1}mol^{-1})	1219	1172	1143	1131	1138	1161

Name: Bis(4–decyloxyphenyl)diazene–1–oxide
Formula: $C_{32}H_{50}N_2O_3$

CAS–RN: 2312–12–1
Group No.: 62–125
Molar Mass: 510.76

TABLE 62.125.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64ARN2	396.5–428.1	13S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	430.0–448.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.125.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	398.1–428.1	11	0.70#	0.637	7.27–1	0.45	–8.86–3	–1
64ARN2	430.0–448.0	5	0.70#	0.123	1.27–1	0.09	3.50–2	1

TABLE 62.125.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	16	0.642	7.32–1	0.45	4.85–3	0

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
398.1–415.0	2.50967+5	–1.81055+5	4.35693+4	–3.49520+3	IV
415.0–448.0	3.00374+3	–1.80442+3	3.76446+2	–2.58909+1	IV

TABLE 62.125.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450
c_p (J K^{-1}g^{-1})	2.668	2.437	2.401	2.389	2.390	2.403
C_p (J K^{-1}mol^{-1})	1363	1245	1226	1220	1221	1227

Name: Bis[4–(undecyloxy)phenyl]diazene–1–oxide
Formula: $C_{34}H_{54}N_2O_3$

CAS–RN: 2312–13–2
Group No.: 62–126
Molar Mass: 538.81

TABLE 62.126.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64ARN2	394.5–428.1	13S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	429.0–441.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.126.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	396.1–428.1	11	0.70#	0.738	8.91–1	0.52	–2.48–2	–3
64ARN2	429.0–441.0	5	0.70#	0.209	2.28–1	0.15	7.68–2	1

TABLE 62.126.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	18	16	0.752	9.05–1	0.53	6.98–3	–2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
396.1–415.0	2.36604+5	–1.71099+5	4.12728+4	–3.31881+3	IV
415.0–441.0	–2.18359+4	1.57250+4	–3.74509+3	2.97085+2	IV

TABLE 62.126.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440
c_p ($J K^{-1} g^{-1}$)	2.596	2.429	2.409	2.394	2.407
C_p ($J K^{-1} mol^{-1}$)	1399	1309	1298	1290	1297

Name: Bis[4–(dodecyloxy)phenyl]diazene–1–oxide
Formula: $C_{36}H_{58}N_2O_3$

CAS–RN: 2312–14–3
Group No.: 62–127
Molar Mass: 566.87

TABLE 62.127.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64ARN2	395.0–428.1	11S	0.30	not specified		C_p	BSAO	64ARN1
64ARN2	429.0–446.0	eqn	0.30	not specified		C_p	BSAO	64ARN1

TABLE 62.127.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
64ARN2	395.6–428.1	10	0.70#	0.842	1.07	0.59	–2.91–2	–2
64ARN2	429.0–446.2	5	0.70#	0.326	3.74–1	0.23	8.78–2	1

TABLE 62.127.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	15	0.873	1.10	0.61	9.86–3	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
395.6–415.0		2.90938+5	–2.10489+5	5.07913+4	–4.08539+3		IV
415.0–446.2		–2.09019+4	1.49374+4	–3.52837+3	2.77636+2		IV

TABLE 62.127.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	2.599	2.420	2.408	2.396	2.398	2.441
C_p ($J K^{-1} mol^{-1}$)	1473	1372	1365	1358	1360	1384

63. Compounds of Carbon, Hydrogen, Oxygen and Sulfur

This is the smallest family as it contains data for 6 compounds only with only one compound measured at one temperature, 303 K.

From an industrial standpoint, dimethylsulfoxide is the most important chemical from this family. Several data points are available for this compound, most of them at 298.15 K, and were obtained from the excess heat capacities measurements. These data suffer from having large experimental uncertainties due to impurities in the samples. The only extensive data set of high quality was that determined at UMAA (70CLE/WES) over a temperature range of 50 K. The same paper also contains data for dimethylsulfone.

Name: Sulfinylbismethane
Formula: C_2H_6OS

CAS-RN: 67-68-5
Group No.: 63-001
Molar Mass: 78.14

TABLE 63.1.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
60KEN/LIN		298.1–343.1	2	nosp	not specified		C_p	BSIO	57KEN
62MUR/YAM	N	315.6	1	nosp	not specified		C_{avg}	not specified	
70CLE/WES		295.8–348.0	12	0.15	99.96	chrom	C_p	BSAO	68WES/FUR
78DEV/HEU		298.1	1	1.00	99.8	chrom	C_p	BSIO	70LKB/COM
79DEV/SOM		298.1	1	1.00	99.8	chrom	C_p	BSIO	70LKB/COM
86KOR/KUK		298.0	1	0.20	not specified		C_p	BSAO	83KUK/KOR
88ROD/MAR	N	298.1	1	nosp	not specified		C_p	BSIO	88ROD/MAR
89BAR/KOO1		298.1	1	nosp	not specified		C_p	FSIT	71PIC/LED
91GRO/ROU		298.1	1	nosp	99.5	anal	C_p	FSIT	71PIC/LED
92MIY/TAM		298.1	1	nosp	99.6	chrom	C_p	FSIO	85OGA

62MUR/YAM average value in temperature range 298–333 K
88ROD/MAR water content 0.009 % (Karl Fisher method)

TABLE 63.1.2. Correlated heat capacities

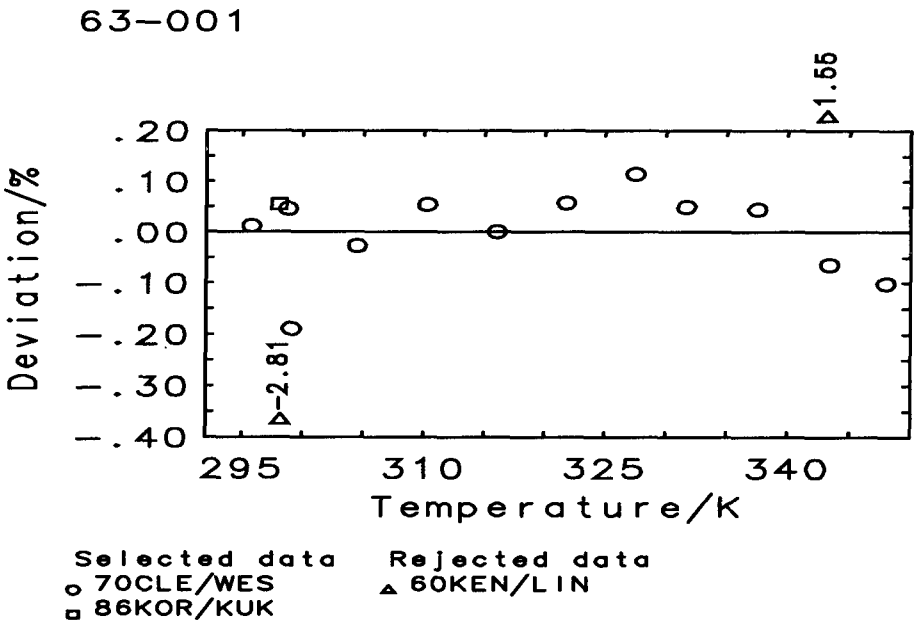
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
70CLE/WES	295.8–348.0	12	0.15	0.534	1.49–2	0.08	–4.31–4	3
86KOR/KUK	298.0	1	0.20	0.264	9.71–3	0.05	9.71–3	1
				Rejected data				
60KEN/LIN	(4.13–1, 2.27,–1.03–1, 0)			62MUR/YAM	(4.58, 19.76, 4.58, 1)			
78DEV/HEU	(3.33–1, 1.77, 3.33–1, 1)			79DEV/SOM	(3.33–1, 1.77, 3.33–1, 1)			
88ROD/MAR	(6.05–2, 0.33, 6.05–2, 1)			89BAR/KOO1	(5.83–1, 3.27, –5.83–1, –1)			
91GRO/ROU	(4.96–1, 2.77,–4.96–1, –1)			92MIY/TAM	(5.87–1, 3.29, –5.87–1, –1)			

TABLE 63.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	22	13	0.564	1.59–2	0.09	3.49–4	4
Temp. range K		A_1	A_2				Level of uncertainty
295.8–348.0		1.50501+1	1.12946				II

TABLE 63.1.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340	350
c_p (J K^{-1}g^{-1})	1.962	1.974	1.986	1.998	2.010	2.022
C_p (J K^{-1}mol^{-1})	153.3	154.2	155.2	156.1	157.1	158.0



Name: Sulfonylbismethane
Formula: $C_2H_6O_2S$

CAS–RN: 67–71–0
Group No.: 63–002
Molar Mass: 94.13

TABLE 63.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70CLE/WES	388.5–414.0	8	0.15	100.00	chrom	C_p	BSAO	68WES/FUR

TABLE 63.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	1.093	3.58–2	0.16	8.75–5	–2
Temp. range K		A_1	A_2				Level of uncertainty
388.5–414.0		1.42422+1	1.88227				III

TABLE 63.2.4. Recommended values of heat capacities

Temp. (K)	390	400	410
c_p ($J K^{-1} g^{-1}$)	1.906	1.923	1.940
C_p ($J K^{-1} mol^{-1}$)	179.5	181.0	182.6

Name: 3–Mercaptopropanoic acid
Formula: $C_3H_6O_2S$

CAS–RN: 107–96–0
Group No.: 63–003
Molar Mass: 106.15

TABLE 63.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
35HUF/ELL	N	299.8–309.9	3	1.00	not specified	C_p	BSIO	25PAR

35HUF/ELL sample contained impurities (premelting)

TABLE 63.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.214	5.26–2	0.21	7.50–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
299.8–309.9		1.49380+1	3.14927				V

TABLE 63.3.4. Recommended values of heat capacities

Temp. (K)	300	310
c_p ($J K^{-1} g^{-1}$)	1.91	1.93
C_p ($J K^{-1} mol^{-1}$)	203	205

Name: Tetrahydrothiophene 1,1–dioxide
Formula: $C_4H_8O_2S$

CAS–RN: 126–33–0
Group No.: 63–004
Molar Mass: 120.17

TABLE 63.4.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69TOM/LIN	303.15	1.306	nosp	not specified		C_p	BSIO	69TOM/LIN

Name: Naphtol[1,8–*cd*]–1,2–dithiole–1–oxide
Formula: $C_{10}H_6O_2S$

CAS–RN: 49833–12–7
Group No.: 63–005
Molar Mass: 190.22

TABLE 63.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75CUC2	373.0–473.0	12S	nosp	not specified		C_{avg}	BDHT	75CUC1

TABLE 63.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	12	12	0.076	1.72–1	0.23	6.48–4	0
Temp. range K		A_1	A_2				Level of uncertainty
373.0–473.0		4.94720+1	6.26690				V

TABLE 63.5.4. Recommended values of heat capacities

Temp. (K)	370	380	390	400	410	420	430
c ($J\,K^{-1}g^{-1}$)	3.18	3.20	3.23	3.26	3.29	3.31	3.34
C ($J\,K^{-1}mol^{-1}$)	604	609	615	620	625	630	635
Temp. (K)	440	450	460	470			
c ($J\,K^{-1}g^{-1}$)	3.37	3.40	3.42	3.45			
C ($J\,K^{-1}mol^{-1}$)	641	646	651	656			

Name: Dibenzo[*c*,*e*][1,2]dithiin–5–oxide
Formula: $C_{12}H_8OS_2$

CAS–RN: 49833–13–8
Group No.: 63–006
Molar Mass: 232.33

TABLE 63.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75CUC2	423.0–523.0	9S	nosp	not specified		C_{avg}	BDHT	75CUC1

TABLE 63.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	9	9	0.069	2.04–1	0.21	8.25–4	1
Temp. range K		A_1	A_2				Level of uncertainty
423.0–523.0		4.96758+1	1.01833+1				V

TABLE 63.6.4. Recommended values of heat capacities

Temp. (K)	420	430	440	450	460	470	480
c ($J K^{-1} g^{-1}$)	3.31	3.34	3.38	3.42	3.45	3.49	3.53
C ($J K^{-1} mol^{-1}$)	769	777	786	794	803	811	819
Temp. (K)	490	500	510	520			
c ($J K^{-1} g^{-1}$)	3.56	3.60	3.64	3.67			
C ($J K^{-1} mol^{-1}$)	828	836	845	853			

64. Miscellaneous Compounds

The miscellaneous family covers compounds that contain atoms of nitrogen, oxygen, sulfur, and halogens in their molecular structures in addition to carbon and hydrogen and have not been treated in descriptions of preceding families. The group contains 30 compounds, 8 of which were measured at one temperature only.

Four fluorinated nitrogen compounds were measured at MSUM (69PAU/LAV3, 71PAU1, 79ZHO/KOS, 80ZHO/KOS). The authors claim these data have an error of 0.3 % but a somewhat higher uncertainty level has been assigned by us. Three derivatives of thiazole of high purity were measured at UMAA (68GOU/WES3, 68GOU/WES4, 69GOU/WES); the uncertainty of these data is small as has been most results reported by this laboratory. The same high quality characteristics regarding uncertainty and purity of compounds also applies to two measurements carried out at BMB/NIPER (63GOO/MES, 92STE/CHI2). For benzothiazole, the excellent agreement between the data from UMAA and NIPER justified assignment of the lowest level of uncertainty (I) to the recommended data obtained by combining the results of adiabatic experiments performed in both laboratories up to a temperature of 320 K.

Trifluoromethanethiol and trifluoroacetonitrile were investigated at WRUC (60DIN/PAC, 61PAC/BOB) and the resulting data showed an error of 0.2 %. A minimum on the $C_{sat} = f(T)$ curves for both compounds was identified and located about 30 and 60 K above the triple point temperature, respectively. A higher uncertainty level (III) has been assigned to trifluoromethanethiol due to the onset of decomposition as the normal boiling temperature 235 K is approached.

Very reliable data for 2-chloro-6-(trichloromethyl)-pyridine originate from a collaboration between DICP and OCUO (87TAN/YE). Two other compounds belonging to the so-called liquid crystals were also measured at OCUO (82TSU/SOR1, 82TSU/SOR2). More information on sources of data for liquid crystals can be found in the introduction to the family of CHNO compounds (group no. 62.).

The data from RAB (78MAR/CIO1) have been considered as highly dubious and have not been used in correlations even when these data were the only source. This was the case in this family for 1-chloro-4-nitrobenzene where we have presented only a reference in the table Experimental Heat Capacities just for completeness of the literature review.

Name: Chlorotrinitromethane
Formula: $CClN_3O_6$

CAS-RN: 1943-16-4
Group No.: 64-001
Molar Mass: 185.48

TABLE 64.1.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64ZIM/BAR	N	298.15	0.8786	nosp	100.0	chrom	C_p	not specified	

64ZIM/BAR temperature not specified; estimated according to other data by the same authors

Name: Trifluoromethanethiol
Formula: CHF_3S

CAS-RN: 1493-15-8
Group No.: 64-002
Molar Mass: 102.08

TABLE 64.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60DIN/PAC	120.8–227.4	39	0.10	not specified		C_{sat}	BSAO	55PAC/PIE

TABLE 64.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	39	39	1.560	2.05–2	0.16	5.82–5	–7
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
120.8–227.4		1.68141+1	–5.90722	2.80496	–3.73317–1		III

TABLE 64.2.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_{sat} (J K^{-1}g^{-1})	1.069	1.063	1.060	1.059	1.060	1.062	1.066
C_{sat} (J K^{-1}mol^{-1})	109.1	108.5	108.2	108.1	108.2	108.5	108.9
Temp. (K)	190	200	210	220	230		
c_{sat} (J K^{-1}g^{-1})	1.072	1.078	1.085	1.093	1.102		
C_{sat} (J K^{-1}mol^{-1})	109.4	110.0	110.8	111.6	112.4		

Name: Trifluoroacetonitrile
Formula: C_2F_3N

CAS–RN: 353–85–5
Group No.: 64–003
Molar Mass: 95.02

TABLE 64.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
61PAC/BOB	131.9–197.0	18	0.10	99.96	melpt	C_{sat}	BSAO	55PAC/PIE

TABLE 64.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	18	18	1.402	2.01–2	0.14	4.73–5	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
131.9–197.0		1.62427+1	–2.05212	5.21869–1			II

TABLE 64.3.4. Recommended values of heat capacities

Temp. (K)	130	140	150	160	170	180	190
c_{sat} (J K^{-1}g^{-1})	1.265	1.259	1.255	1.251	1.248	1.246	1.245
C_{sat} (J K^{-1}mol^{-1})	120.2	119.7	119.2	118.9	118.6	118.4	118.3
Temp. (K)	200						
c_{sat} (J K^{-1}g^{-1})	1.245						
C_{sat} (J K^{-1}mol^{-1})	118.3						

Name: Thiazole
Formula: C_3H_3NS

CAS–RN: 288–47–1
Group No.: 64–004
Molar Mass: 85.13

TABLE 64.4.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
68GOU/WES4	N	244.6–336.6	14	0.10	99.91	melpt	C_{sat}	BSAO	68WES/FUR

68GOU/WES4 smoothed values in 68GOU/WES1 and 69SOU/GOU1

TABLE 64.4.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	13	1.886	2.65–2	0.19	5.99–5	4

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
244.8–290.0	2.31344+1	–1.30831+1	5.37207	–6.53329–1	II
290.0–336.6	–1.82933+2	2.00090+2	–6.81360+1	7.79587	II

TABLE 64.4.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.333	1.347	1.363	1.378	1.383	1.394	1.410
C_{sat} (J K^{-1}mol^{-1})	113.5	114.7	116.0	117.3	117.8	118.7	120.0
Temp. (K)	298.15	300	310	320	330	340	
c_{sat} (J K^{-1}g^{-1})	1.423	1.426	1.446	1.475	1.516	1.575	
C_{sat} (J K^{-1}mol^{-1})	121.1	121.4	123.1	125.5	129.1	134.1	

TABLE 64.4.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	14	13	4.565	6.70–2	0.46	4.88–4	–1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
244.9–336.6	629.00	6.61387+1	2.80151+1	–1.46956+1	3.90354+1	III

Name: Isothiocyanatoethane
Formula: C_3H_5NS

CAS–RN: 542–85–8
Group No.: 64–005
Molar Mass: 87.15

TABLE 64.5.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36KUR/VOS	N	312.15	1.222	nosp	not specified		C_{avg}	DSIO	36KUR/VOS

36KUR/VOS average value in temperature range 290–333 K

Name: *N,N,N',N'*–Tetrafluoro–1,2–propanediamine
Formula: $C_3H_6F_4N_2$

CAS–RN: 15403–25–5
Group No.: 64–006
Molar Mass: 146.09

TABLE 64.6.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70REE/SEE	N	298.15	1.456	1.50	99.	chrom	C_p	DSIO	64EDI/CUB

70REE/SEE same datum in 68REE/SEE

Name: *O*–Methyl ester 2,3,3–trichloro–2–propenethioic acid
Formula: $C_4H_3Cl_3OS$

CAS–RN: 76619–91–5
Group No.: 64–007
Molar Mass: 205.49

TABLE 64.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80SHA/LYU	286.0–330.0	7S	0.50	99.07	melpt	C_p	BSAO	80SHA/LYU

TABLE 64.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.028	4.15–3	0.01	–5.45–7	–1

Temp. range K	A_1	A_2	Level of uncertainty
286.0–330.0	2.86286+1	2.77341–1	IV

TABLE 64.7.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p ($J\,K^{-1}g^{-1}$)	1.191	1.192	1.192	1.193	1.194	1.195
C_p ($J\,K^{-1}mol^{-1}$)	244.7	244.9	245.0	245.2	245.4	245.6

Name: 3–Isothiocyanato–1–propene
Formula: C_4H_5NS

CAS–RN: 57–06–7
Group No.: 64–008
Molar Mass: 99.16

TABLE 64.8.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
36KUR/VOS	N	311.65	1.552	nosp	not specified		C_{avg}	DSIO	36KUR/VOS

36KUR/VOS average value in temperature range 290–333 K

Name: 2–Methylthiazole
Formula: C_4H_5NS

CAS–RN: 3581–87–1
Group No.: 64–009
Molar Mass: 99.16

TABLE 64.9.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
68GOU/WES3	N	259.9–340.6	13	0.10	99.902	melpt	C_{sat}	BSAO	68WES/FUR

68GOU/WES3 smoothed values in 68GOU/WES2 and 69SOU/GOU2

TABLE 64.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	13	13	1.254	2.32–2	0.13	2.93–5	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
259.9–340.6	–3.33732+1	5.08581+1	–1.74519+1	2.07545	II

TABLE 64.9.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J $K^{-1}g^{-1}$)	1.456	1.473	1.479	1.490	1.506	1.520	1.524
C_{sat} (J $K^{-1}mol^{-1}$)	144.4	146.1	146.6	147.7	149.4	150.8	151.1

Temp. (K)	310	320	330	340
c_{sat} (J $K^{-1}g^{-1}$)	1.543	1.566	1.593	1.625
C_{sat} (J $K^{-1}mol^{-1}$)	153.0	155.3	157.9	161.1

TABLE 64.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	13	13	1.683	3.06–2	0.17	8.01–5	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
259.9–340.6	646.00	2.23008+1	1.37479+1	2.23019	9.04369	II

Name: Undecafluoropiperidine
Formula: $C_5F_{11}N$

CAS–RN: 836–77–1
Group No.: 64–010
Molar Mass: 283.04

TABLE 64.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63GOO/TOD	279.3–319.0	11	0.20	99.49	melpt	C_{sat}	BSAO	47HUF

TABLE 64.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	11	11	0.104	7.42–3	0.02	2.43–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
279.3–319.0		1.78018+1	6.00217				II

TABLE 64.10.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_{sat} (J K^{-1}g^{-1})	1.017	1.034	1.049	1.052	1.070	1.087
C_{sat} (J K^{-1}mol^{-1})	287.7	292.7	296.8	297.7	302.7	307.7

Name: 1,1,2,2,2–Pentafluoro–*N*–(pentafluoroethyl)–*N*–(trifluoromethyl)–ethanamine
Formula: $C_5F_{13}N$

CAS–RN: 758–48–5
Group No.: 64–011
Molar Mass: 321.04

TABLE 64.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
80ZHO/KOS	149.4–297.4	27	nosp	97.7	melpt	C_{sat}	BSAO	79ZHO/KOS

TABLE 64.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	27	27	0.467	4.94–2	0.14	1.13–4	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
149.4–297.4		9.14714	2.24644+1	–6.36550	7.96286–1		IV

TABLE 64.11.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_{sat} (J K^{-1}g^{-1})	0.808	0.830	0.851	0.870	0.889	0.906	0.923
C_{sat} (J K^{-1}mol^{-1})	259.5	266.5	273.2	279.4	285.3	290.9	296.2
Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	0.939	0.954	0.969	0.983	0.998	1.012	1.016
C_{sat} (J K^{-1}mol^{-1})	301.3	306.2	311.0	315.7	320.3	324.8	326.3
Temp. (K)	280	290	298.15	300			
c_{sat} (J K^{-1}g^{-1})	1.026	1.041	1.053	1.055			
C_{sat} (J K^{-1}mol^{-1})	329.4	334.1	337.9	338.8			

Name: Pentafluoronitrobenzene
Formula: $C_6F_5NO_2$

CAS–RN: 880–78–4
Group No.: 64–012
Molar Mass: 213.06

TABLE 64.12.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
71PAU1	N	249.7–300.0	8S	nosp	not specified		C_{sat}	BSAO	69PAU/LAV2

71PAU1 measured data deposited in VINITI No 2537–71

TABLE 64.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	8	8	0.091	1.18–2	0.04	4.53–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
249.7–300.0		2.73927+1	1.81743				III

TABLE 64.12.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	1.246	1.253	1.260	1.263	1.268	1.275	1.280
C_{sat} (J K^{-1}mol^{-1})	265.5	267.0	268.6	269.0	270.1	271.6	272.8
Temp. (K)	300						
c_{sat} (J K^{-1}g^{-1})	1.282						
C_{sat} (J K^{-1}mol^{-1})	273.1						

Name: 1,1,2,2,2–Pentafluoro–*N*,*N*–bis(pentafluoroethyl)ethanamine
Formula: $C_6F_{15}N$

CAS–RN: 359–70–6
Group No.: 64–013
Molar Mass: 371.05

TABLE 64.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79ZHO/KOS	160.0–300.0	31S	nosp	99.07	melpt	C_{sat}	BSAO	79ZHO/KOS

TABLE 64.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	31	31	0.109	1.78–2	0.04	1.23–5	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
160.0–300.0		1.83414+1	1.66726+1	–4.20332	5.64732–1		III

TABLE 64.13.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_{sat} (J K^{-1}g^{-1})	0.819	0.836	0.852	0.868	0.883	0.897	0.912
C_{sat} (J K^{-1}mol^{-1})	304.1	310.2	316.2	321.9	327.5	333.0	338.3
Temp. (K)	230	240	250	260	270	273.15	280
c_{sat} (J K^{-1}g^{-1})	0.926	0.940	0.954	0.968	0.982	0.987	0.996
C_{sat} (J K^{-1}mol^{-1})	343.6	348.8	354.0	359.2	364.4	366.1	369.7
Temp. (K)	290	298.15	300				
c_{sat} (J K^{-1}g^{-1})	1.011	1.023	1.026				
C_{sat} (J K^{-1}mol^{-1})	375.1	379.6	380.6				

Name: 2,3,4,5,6–Pentafluorobenzenamine
Formula: $C_6H_2F_5N$

CAS–RN: 771–60–8
Group No.: 64–014
Molar Mass: 183.08

TABLE 64.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69PAU/LAV3	309.7–317.8	5	nosp	99.36	melpt	C_{sat}	BSAO	69PAU/LAV2

TABLE 64.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	5	5	0.396	4.88–2	0.16	9.35–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
309.7–317.8		2.90487+1	5.68823–1				III

TABLE 64.14.4. Recommended values of heat capacities

Temp. (K)	310	320
c_{sat} (J K^{-1}g^{-1})	1.399	1.402
C_{sat} (J K^{-1}mol^{-1})	256.2	256.7

Name: 2–Chloro–6–(trichloromethyl)pyridine
Formula: $C_6H_3Cl_4N$

CAS–RN: 1929–82–4
Group No.: 64–015
Molar Mass: 230.91

TABLE 64.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87TAN/YE	337.0–400.0	8S	nosp	99.95	chrom	C_p	BSAO	83TAN/ZHO

TABLE 64.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.011	1.66–3	0.01	–4.77–7	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
337.0–400.0	9.00189	1.07621+1	–1.25187	III

TABLE 64.15.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390	400
c_p ($J\,K^{-1}g^{-1}$)	1.121	1.128	1.135	1.141	1.146	1.150	1.153
C_p ($J\,K^{-1}mol^{-1}$)	258.8	260.5	262.1	263.4	264.6	265.5	266.2

Name: 1–Bromo–3–nitrobenzene
Formula: $C_6H_4BrNO_2$

CAS–RN: 585–79–5
Group No.: 64–016
Molar Mass: 202.01

TABLE 64.16.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
08BOG/WIN	N	340.15	1.109	nosp	not specified		C_{avg}	DSIO	08BOG/WIN

08BOG/WIN average value in temperature range 327–353 K

Name: 1–Chloro–3–nitrobenzene
Formula: $C_6H_4ClNO_2$

CAS–RN: 121–73–3
Group No.: 64–017
Molar Mass: 157.56

TABLE 64.17.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
08BOG/WIN	N	338.15	1.402	nosp	not specified		C_{avg}	DSIO	08BOG/WIN

08BOG/WIN average value in temperature range 318–358 K

Name: 1–Chloro–4–nitrobenzene
Formula: $C_6H_4ClNO_2$

CAS–RN: 100–00–5
Group No.: 64–018
Molar Mass: 157.56

TABLE 64.18.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78MAR/CIO1	N	354.6–466.9	2	nosp	not specified		C_p	DSIO	71MAR/CIO

78MAR/CIO1 constant value calculated from temperature dependence of enthalpy by the authors

TABLE 64.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
354.6–466.9		2.88600+1					VI

TABLE 64.18.4. Recommended values of heat capacities

Temp. (K)	360	410	460
c_p ($J\,K^{-1}g^{-1}$)	1.52	1.52	1.52
C_p ($J\,K^{-1}mol^{-1}$)	240	240	240

Name: 3–Chlorobenzenamine
Formula: C_6H_6ClN

CAS–RN: 108–42–9
Group No.: 64–019
Molar Mass: 127.57

TABLE 64.19.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
65ZAL/KOC	N	294.6–323.1	2	nosp	99.	estim	C_p	not specified	

65ZAL/KOC technical product, purity in question

TABLE 64.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
294.6–323.1		1.25983+1	3.82928				VI

TABLE 64.19.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	1.54	1.57	1.57	1.59	1.62
C_p ($J K^{-1}mol^{-1}$)	197	200	200	203	207

Name: 4–Fluorobenzenamine
Formula: C_6H_6FN

CAS–RN: 371–40–4
Group No.: 64–020
Molar Mass: 111.12

TABLE 64.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
91LIC	N	224.0–337.0	eqn	2.00	99.0	anal	C_p	BDCT	89BRE/LIC

91LIC low temperature limit is below n.m.t.; undercooled liquid

TABLE 64.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.000	1.35–6	0.00	–6.68–7	0

Temp. range K	A_1	A_2	Level of uncertainty
224.0–336.1	2.01832+1	1.10650	V

TABLE 64.20.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.70	1.71	1.72	1.73	1.73	1.74	1.74
C_p ($J K^{-1}mol^{-1}$)	189	190	191	192	193	193	194
Temp. (K)	290	298.15	300	310	320	330	340
c_p ($J K^{-1}g^{-1}$)	1.75	1.76	1.76	1.77	1.78	1.78	1.79
C_p ($J K^{-1}mol^{-1}$)	194	195	195	196	197	198	199

Name: 1–Chloro–3–isocyanatobenzene
Formula: C_7H_4ClNO

CAS–RN: 2909–38–8
Group No.: 64–021
Molar Mass: 153.57

TABLE 64.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
65ZAL/KOC	N	294.1–323.1	2	nosp	99.	estim	C_p	not specified	

65ZAL/KOC technical product, purity in question

TABLE 64.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
294.1–323.1		1.07303+1	3.99712				VI

TABLE 64.21.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	1.21	1.23	1.23	1.25	1.27
C_p ($J K^{-1}mol^{-1}$)	186	188	189	192	196

Name: 1–Nitro–3–(trifluoromethyl)benzene
Formula: $C_7H_4F_3NO_2$

CAS–RN: 98–46–4
Group No.: 64–022
Molar Mass: 191.11

TABLE 64.22.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
81LEB/RYA	N	335.50	1.172	1.00	not specified		C_{avg}	DSIO	76LEB/RYA

81LEB/RYA average value in temperature range 298–373 K

Name: Benzothiazole
Formula: C_7H_5NS

CAS–RN: 95–16–9
Group No.: 64–023
Molar Mass: 135.19

TABLE 64.23.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
69GOU/WES	N	279.0–319.4	14	0.10	99.91	melpt	C_p	BSAO	68WES/FUR
92STE/CHI2		282.2–441.0	18	0.10	99.99	melpt	C_{sat}	BSAO	47HUF
92STE/CHI2		320.0–600.0	15	nosp	99.99	melpt	C_{sat}	BDHT	89KNI/ARC

69GOU/WES smoothed values in 68GOU/WES3

TABLE 64.23.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
69GOU/WES	279.0–319.4	14	0.10	1.257	2.86–2	0.13	1.03–2	5
92STE/CHI2	282.2–441.0	17	0.10	0.557	1.28–2	0.06	–8.66–3	–8
92STE/CHI2	320.0–600.0	15	1.00#	0.324	9.79–2	0.32	2.51–2	2

TABLE 64.23.3. Parameters of cubic spline polynomials

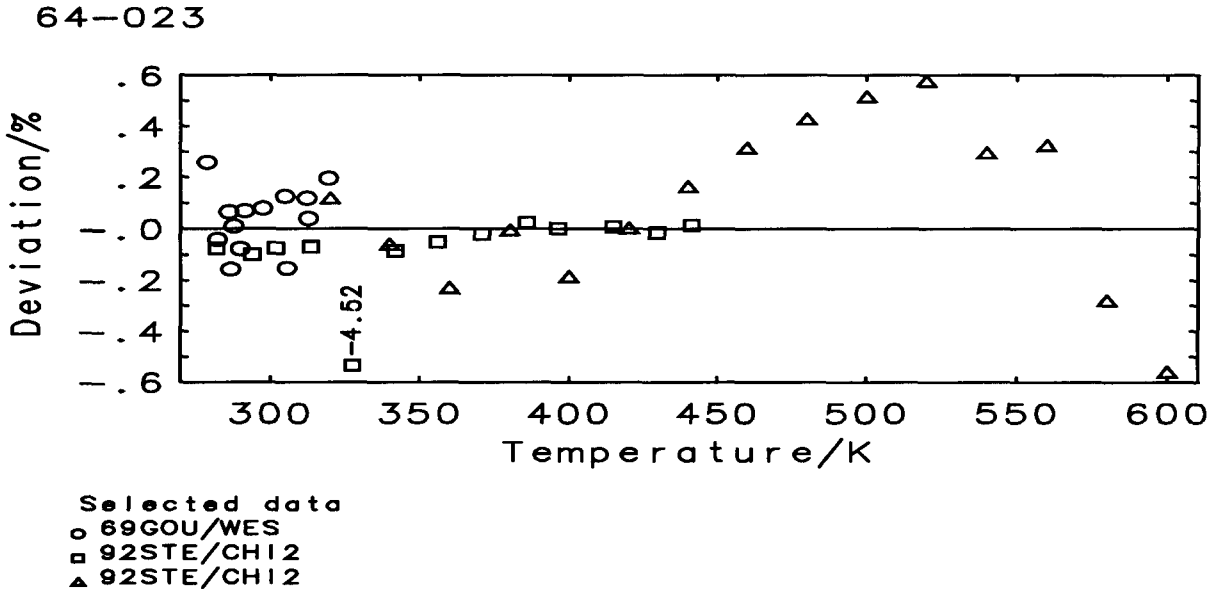
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	47	46	0.841	6.21–2	0.21	8.13–3	–1
C_{sat}	47	46	0.844	6.40–2	0.22	8.20–3	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
279.0–320.0		4.11628+1	–2.30272+1	8.20630	–8.55542–1		I
320.0–600.0		1.23684+1	3.96757	–2.29578–1	2.31946–2		IV
279.0–320.0		3.95471+1	–2.14587+1	7.70023	–8.01285–1		I
320.0–600.0		1.28671+1	3.55378	–1.16164–1	1.29228–2		IV

TABLE 64.23.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.3680	1.3858	1.4011	1.4046	1.4240	1.4437	1.463
C_p ($J K^{-1} mol^{-1}$)	184.94	187.35	189.41	189.89	192.51	195.17	197.8
c_{sat} ($J K^{-1} g^{-1}$)	1.3680	1.3859	1.4011	1.4046	1.4240	1.4437	1.463
C_{sat} ($J K^{-1} mol^{-1}$)	184.94	187.35	189.41	189.89	192.51	195.17	197.8
Temp. (K)	340	350	360	370	380	390	400
c_p ($J K^{-1} g^{-1}$)	1.483	1.503	1.523	1.543	1.562	1.582	1.602
C_p ($J K^{-1} mol^{-1}$)	200.5	203.2	205.9	208.5	211.2	213.9	216.6
c_{sat} ($J K^{-1} g^{-1}$)	1.483	1.503	1.523	1.543	1.562	1.582	1.602
C_{sat} ($J K^{-1} mol^{-1}$)	200.5	203.2	205.9	208.5	211.2	213.9	216.6
Temp. (K)	410	420	430	440	450	460	470
c_p ($J K^{-1} g^{-1}$)	1.622	1.642	1.662	1.683	1.703	1.723	1.744
C_p ($J K^{-1} mol^{-1}$)	219.3	222.0	224.7	227.5	230.2	233.0	235.7
c_{sat} ($J K^{-1} g^{-1}$)	1.622	1.642	1.662	1.682	1.703	1.723	1.743
C_{sat} ($J K^{-1} mol^{-1}$)	219.3	222.0	224.7	227.4	230.2	232.9	235.7
Temp. (K)	480	490	500	510	520	530	540
c_p ($J K^{-1} g^{-1}$)	1.764	1.785	1.806	1.827	1.848	1.870	1.891
C_p ($J K^{-1} mol^{-1}$)	238.5	241.3	244.2	247.0	249.9	252.8	255.7
c_{sat} ($J K^{-1} g^{-1}$)	1.764	1.784	1.805	1.826	1.846	1.867	1.888
C_{sat} ($J K^{-1} mol^{-1}$)	238.4	241.2	244.0	246.8	249.6	252.5	255.3
Temp. (K)	550	560	570	580	590	600	
c_p ($J K^{-1} g^{-1}$)	1.913	1.935	1.957	1.979	2.002	2.025	
C_p ($J K^{-1} mol^{-1}$)	258.6	261.6	264.6	267.6	270.6	273.7	
c_{sat} ($J K^{-1} g^{-1}$)	1.910	1.931	1.952	1.974	1.995	2.017	
C_{sat} ($J K^{-1} mol^{-1}$)	258.2	261.0	263.9	266.8	269.8	272.7	

TABLE 64.23.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R		s_r %	s_b/R	+/–
C_p	47	46	0.917	7.01–2		0.23	6.62–3	12
Temp. range K	T_c K	A_1	A_2	A_3	A_4			Level of uncertainty
279.0–600.0	771.00	–1.87516	4.19472–2	1.37022+1	2.09563+1			IV



Name: Isothiocyanatobenzene
Formula: C_7H_5NS

CAS-RN: 103-72-0
Group No.: 64-024
Molar Mass: 135.19

TABLE 64.24.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
36KUR/VOS	N	311.65	1.377	nosp	not specified		C_{avg}	DSIO	36KUR/VOS

36KUR/VOS average value in temperature range 290–333 K

Name: Dipropylcarbamic chloride
Formula: $C_7H_{14}ClNO$

CAS-RN: 27086-19-7
Group No.: 64-025
Molar Mass: 163.65

TABLE 64.25.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81LEB/RYA	N	320.5–335.5	2	1.00	99.8	chrom	C_{avg}	DSIO	76LEB/RYA

81LEB/RYA average values in temperature ranges 298–343 K and 298–373 K

TABLE 64.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
320.5–335.5		2.09711+1	4.89102				V

TABLE 64.25.4. Recommended values of heat capacities

Temp. (K)	320	330	340
c ($J K^{-1}g^{-1}$)	1.86	1.89	1.91
C ($J K^{-1}mol^{-1}$)	304	309	313

Name: *S*–Ethyl ester dipropylcarbamothionic acid
Formula: $C_9H_{19}NOS$

CAS–RN: 759–94–4
Group No.: 64–026
Molar Mass: 189.32

TABLE 64.26.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
81LEB/RYA	N	340.5–385.5	2	1.00	not specified	C_{avg}	DSIO	76LEB/RYA

81LEB/RYA average values in temperature ranges 298–383 K and 298–473 K

TABLE 64.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
340.5–385.5		4.27433+1	1.04236				V

TABLE 64.26.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390
c ($J K^{-1}g^{-1}$)	2.03	2.04	2.04	2.05	2.05	2.06
C ($J K^{-1}mol^{-1}$)	385	386	387	387	388	389

Name: 1,1'–Sulfonylbis(4–chlorobenzene)
Formula: $C_{12}H_8Cl_2O_2S$

CAS–RN: 80–07–9
Group No.: 64–027
Molar Mass: 287.17

TABLE 64.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85NOV/TSV	440.0–443.0	2	5.00	not specified		C_p	BDHT	74DSM/COM

TABLE 64.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
440.0–443.0		3.29947+1	4.00903				VI

TABLE 64.27.4. Recommended values of heat capacities

Temp. (K)	440	443
c_p (J $K^{-1}g^{-1}$)	1.47	1.47
C_p (J $K^{-1}mol^{-1}$)	421	422

Name: 4,4'–Sulfonylbisbenzenamine
Formula: $C_{12}H_{12}N_2O_2S$

CAS–RN: 80–08–0
Group No.: 64–028
Molar Mass: 248.31

TABLE 64.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87LES/LIC	460.0–495.0	eqn	2.00	99.	estim	C_p	BDHT	69PER/COM

TABLE 64.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.000	3.48–6	0.00	4.77–7	0
Temp. range K		A_1	A_2				Level of uncertainty
460.0–495.0		3.98245+1	4.30530				V

TABLE 64.28.4. Recommended values of heat capacities

Temp. (K)	460	470	480	490	500
c_p ($J K^{-1}g^{-1}$)	2.00	2.01	2.03	2.04	2.05
C_p ($J K^{-1}mol^{-1}$)	496	499	503	507	510

Name: 4–Chloro–*N*–[[4–(hexyloxy)phenyl]methylene]benzenamine
Formula: $C_{19}H_{22}ClNO$

CAS–RN: 5219–48–7
Group No.: 64–029
Molar Mass: 315.84

TABLE 64.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
82TSU/SOR1	371.1–383.3	9	nosp	not specified		C_p	BSAO	83YOS/SOR1

TABLE 64.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	9	9	0.484	1.11–1	0.15	3.10–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
371.1–383.3		1.48607+3	–7.37897+2	9.65233+1			III

TABLE 64.29.4. Recommended values of heat capacities

Temp. (K)	371	375	379	383
c_p ($J K^{-1}g^{-1}$)	2.028	2.009	1.998	1.996
C_p ($J K^{-1}mol^{-1}$)	640.4	634.5	631.1	630.3

Name: 4–Fluoro–*N*–[[4–(hexyloxy)]methylene]benzenamine
Formula: $C_{19}H_{22}FNO$

CAS–RN: 56544–26–4
Group No.: 64–030
Molar Mass: 299.39

TABLE 64.30.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
82TSU/SOR2	336.6–385.7	33	nosp	99.96	melpt	C_p	BSAO	83YOS/SOR1

TABLE 64.30.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	33	1.685	3.91–1	0.51	3.47–3	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
336.6–342.0		1.54039+6	–1.35099+6	3.94980+5	–3.84929+4		III
342.0–385.7		2.29712+3	–1.78672+3	4.76633+2	–4.22250+1		III

TABLE 64.30.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370	380	390
c_p ($J K^{-1} g^{-1}$)	2.023	1.998	2.001	2.014	2.033	2.048
C_p ($J K^{-1} mol^{-1}$)	605.7	598.3	599.0	603.1	608.6	613.2

7. Organic Compounds Containing other Elements than Halogens, Nitrogen, Oxygen and Sulfur

71. Organosilicon Compounds

The organosilicon family contains 56 compounds, three of which were measured at one temperature (298.15 K) only. This family includes some compounds that contain atoms of halogens, nitrogen, or oxygen in addition to carbon, hydrogen, and silicon atoms.

The majority of compounds in the family (36) were measured at ANAZ which resulted in the publication of a considerable number of articles. However, most of the publications are not easily accessible because they appear mostly in Azerbaidzhanian journals or are deposited in "VINITI" (fSU). Measurements were carried out during the period from 1967 to 1987 using a classical adiabatic calorimeter described in the reference (54STR/ICK). The number of measurements performed over a period of two decades is impressive; however, the uncertainty of the data is probably much worse than the claimed error of 0.3 %. It is difficult to make any qualified estimate of the uncertainty as the authors present only parameters of a smoothing equation without offering any analysis of the raw values. An exception to this is found in the two references: (87DZH/KUL2, 87DZH/KUL3). For three organosilicon compounds, the data are presented only as graphs (75GUS/KAR, 82KUL/DZH); the authors of the last referenced paper provided us kindly with the raw experimental data for 2,2,4,4-tetramethyl-6,6-diphenylcyclotrisiloxane and 2,2-dimethyl-4,4,6,6-tetraphenylcyclotrisiloxane. Comparison with the data obtained in other laboratories was possible only for two compounds. First, the ANAZ results for hexamethyldisiloxane could be compared with the high precision values from BMB (61SCO/MES) and from OSU (75PED/KEY). For these two sources, in general, agreement prevailed among the data. However, the ANAZ data (86DZH/KUL) were found to be on the average 15 % higher compared to the other two sources. Secondly, the ANAZ values (85DZH/KUL) for hexaethylcyclotrisiloxane are higher by 8 % compared to the results from CIUG (82KUL/LEB), which we considered as more credible. The amount of impurities in the compounds measured at ANAZ (if indicated at all) is 1 to 3 %. Because of the above circumstances, the data from ANAZ have been assigned the level of uncertainty V or VI and were discarded in the above two cases because other experimental values were available.

Eight compounds were measured at CIUG (72MAS/RAB, 73LEB/TSV, 74LEB/ARO, 74LEB/TSV, 74MIL/LEB, 77LEB/RAB1, 79LEB/LEB2, 82KUL/LEB) and results showed an uncertainty between 0.3 to 0.5 %; this seems to be reasonable.

An extensive data set of good quality for tetraoxysilane was published by researchers from SUU and Netherlands Energy Research Foundation ECN, Petten (92VAN/COR). For tetramethylsilane, three low temperature data points of good quality from NCLT (73SHI/ENO) were merged with the data from OCUO (77HAR/ATA) available over a wide temperature interval extending up to the normal boiling temperature. Older data for this compound from PSC (41AST/KEN) have been rejected from the correlation as they differed considerably when the normal boiling temperature is approached.

Experimental data for five compounds (purity around 99.5 %) were published by the authors from an unidentified Moscow laboratory (65GUM/KOS1, 65GUM/KOS2, 65GUM/KOS3, 68KOS/MOS, 75KOS/SAM). Due to the large scatter of these data, a high level of uncertainty has been assigned.

In this family, temperature ranges of the experimental data are usually limited and auxiliary data are lacking. For these reasons, the parameters of the quasi-polynomial equation were calculated for four compounds only (tetramethyl silane, tetraethylsilane, hexamethyldisiloxane and tetraethyl ester silicic acid) and no conversion of C_{sat} to C_p data was performed.

Name: Trichloroethenylsilane
Formula: $C_2H_3Cl_3Si$

CAS-RN: 75-94-5
Group No.: 71-001
Molar Mass: 161.49

TABLE 71.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65GUM/KOS2	188.8–300.2	74	nosp	99.43	melpt	C_p	BSAO	54STR/ICK

TABLE 71.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	74	74	0.991	2.88–1	1.49	8.21–3	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
188.8–300.2		2.53268+1	–6.92618	1.85975			V

TABLE 71.1.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	0.97	0.97	0.98	0.98	0.99	1.00	1.01
C_p (J K^{-1}mol^{-1})	157	157	158	159	160	161	163
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.02	1.04	1.04	1.06	1.08	1.09	1.10
C_p (J K^{-1}mol^{-1})	165	168	169	171	174	176	177

Name: Trichloroethylsilane
Formula: $C_2H_5Cl_3Si$

CAS-RN: 115-21-9
Group No.: 71-002
Molar Mass: 163.51

TABLE 71.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69NAG/DZH1	165.3–298.2	15S	nosp	98.99	melpt	C_p	BSAO	54STR/ICK

TABLE 71.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.219	2.47–2	0.11	3.89–5	–1
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
165.3–298.2	1.90127+1	–1.19300	2.02478	–3.89537–1			IV

TABLE 71.2.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.064	1.076	1.087	1.099	1.110	1.121	1.131
C_p (J K^{-1}mol^{-1})	174.0	175.9	177.8	179.7	181.5	183.3	184.9
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.140	1.149	1.157	1.164	1.166	1.169	1.174
C_p (J K^{-1}mol^{-1})	186.5	187.9	189.2	190.3	190.6	191.2	191.9
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.176	1.177					
C_p (J K^{-1}mol^{-1})	192.3	192.4					

Name: Dichloroethylsilane
Formula: $C_2H_6Cl_2Si$

CAS-RN: 1789-58-8
Group No.: 71-003
Molar Mass: 129.06

TABLE 71.3.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69NAG/DZH2	N	170.6–298.2	19S	nosp	98.85	melpt	C_p	BSAO	54STR/ICK

69NAG/DZH2 misprinted C_p at 270 K, correct value 39.41 cal/(K.mol)

TABLE 71.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	19	19	0.090	8.65–3	0.05	6.53–6	1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
170.6–298.2	2.02233+1	–4.17056	2.50411	–3.74606–1	IV

TABLE 71.3.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.201	1.209	1.218	1.227	1.236	1.245	1.254
C_p (J K^{-1}mol^{-1})	155.0	156.1	157.2	158.3	159.5	160.6	161.8
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.262	1.271	1.278	1.281	1.286	1.292	1.296
C_p (J K^{-1}mol^{-1})	162.9	164.0	165.0	165.3	165.9	166.7	167.3
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.297						
C_p (J K^{-1}mol^{-1})	167.4						

Name: 3-Trichlorosilylpropanenitrile
Formula: $C_3H_4Cl_3NSi$

CAS-RN: 1071-22-3
Group No.: 71-004
Molar Mass: 188.52

TABLE 71.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75KOS/SAM	314.4–322.5	6	nosp	99.67	melpt	C_{sat}	BSAO	54STR/ICK

TABLE 71.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	6	6	0.224	1.84–2	0.07	1.53–5	0

Temp. range K	A_1	A_2	Level of uncertainty
314.4–322.5	2.22819+1	1.60314	IV

TABLE 71.4.4. Recommended values of heat capacities

Temp. (K)	310	320
c_{sat} (J K^{-1}g^{-1})	1.202	1.209
C_{sat} (J K^{-1}mol^{-1})	226.6	227.9

Name: 3-(Dichloromethylsilyl)propanenitrile
Formula: $C_4H_7Cl_2NSi$

CAS-RN: 1071-21-2
Group No.: 71-005
Molar Mass: 168.10

TABLE 71.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69KAR/KOS	254.5–300.0	7S	0.20	99.2	melpt	C_p	BSAO	54STR/ICK

TABLE 71.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.236	1.34–2	0.05	1.01–5	–1

Temp. range K	A_1	A_2	Level of uncertainty
254.5–300.0	2.48596+1	1.22541	IV

TABLE 71.5.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.387	1.393	1.395	1.399	1.405	1.410	1.411
C_p (J K^{-1}mol^{-1})	233.2	234.2	234.5	235.2	236.2	237.1	237.3

Name: Dichlordiethylsilane
Formula: $C_4H_{10}Cl_2Si$

CAS-RN: 1719-53-5
Group No.: 71-006
Molar Mass: 157.11

TABLE 71.6.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69NAG/DZH1	N	174.9–300.0	15S	0.20	98.97	melpt	C_p	BSAO	54STR/ICK

69NAG/DZH1 same data in 69KAR/KOS

TABLE 71.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	15	15	0.353	1.76–2	0.07	1.72–5	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
174.9–300.0	2.00879+1	3.75814	–1.27414	2.21076–1	IV

TABLE 71.6.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.271	1.278	1.285	1.292	1.299	1.306	1.314
C_p (J K^{-1}mol^{-1})	199.7	200.8	201.8	202.9	204.1	205.2	206.4
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.322	1.330	1.339	1.342	1.348	1.358	1.367
C_p (J K^{-1}mol^{-1})	207.6	209.0	210.3	210.8	211.8	213.4	214.7
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.369						
C_p (J K^{-1}mol^{-1})	215.0						

Name: Tetramethyl ester silicic acid
Formula: $C_4H_{12}O_4Si$

CAS-RN: 681-84-5
Group No.: 71-007
Molar Mass: 152.22

TABLE 71.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
08KAH/KOE N	342.1	1	nosp	not specified	C_{avg}	DSIO	01KAH
85NKI/CHA	298.0	1	0.30	not specified	C_p	FSIT	71PIC/LED

08KAH/KOE average value in temperature range 296–388 K

TABLE 71.7.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
08KAH/KOE	342.1	1	3.00#	0.000	3.82–6	0.00	–3.82–6	0
85NKI/CHA	298.0	1	0.30	0.000	1.91–6	0.00	–1.91–6	0

TABLE 71.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	–2.86–6	0
Temp. range K		A_1	A_2				Level of uncertainty
298.0–342.1		–3.49120+1	2.14224+1				V

TABLE 71.7.4. Recommended values of heat capacities

Temp. (K)	300	310	320	330	340
c_p (J K^{-1}g^{-1})	1.60	1.72	1.84	1.95	2.07
C_p (J K^{-1}mol^{-1})	244	262	280	298	315

Name: Tetramethylsilane
Formula: $C_4H_{12}Si$

CAS–RN: 75–76–3
Group No.: 71–008
Molar Mass: 88.22

TABLE 71.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
41AST/KEN	176.9–293.5	22	nosp	99.89	melpt	C_p	BSIO	36AST/MES
73SHI/ENO	176.0–177.4	3	nosp	99.995	melpt	C_p	BSAO	73SHI/ENO
77HAR/ATA	175.5–297.5	43	nosp	99.986	melpt	C_p	BSAO	74ATA/CHI

TABLE 71.8.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73SHI/ENO	176.0–177.4	3	0.20#	0.274	1.08–2	0.05	7.44–3	1
77HAR/ATA	175.5–297.5	43	0.50#	1.011	1.13–1	0.51	–2.09–3	–7
				Rejected data				
41AST/KEN	(3.68–1, 1.55, 2.05–1, 16)							

TABLE 71.8.3. Parameters of regression polynomial

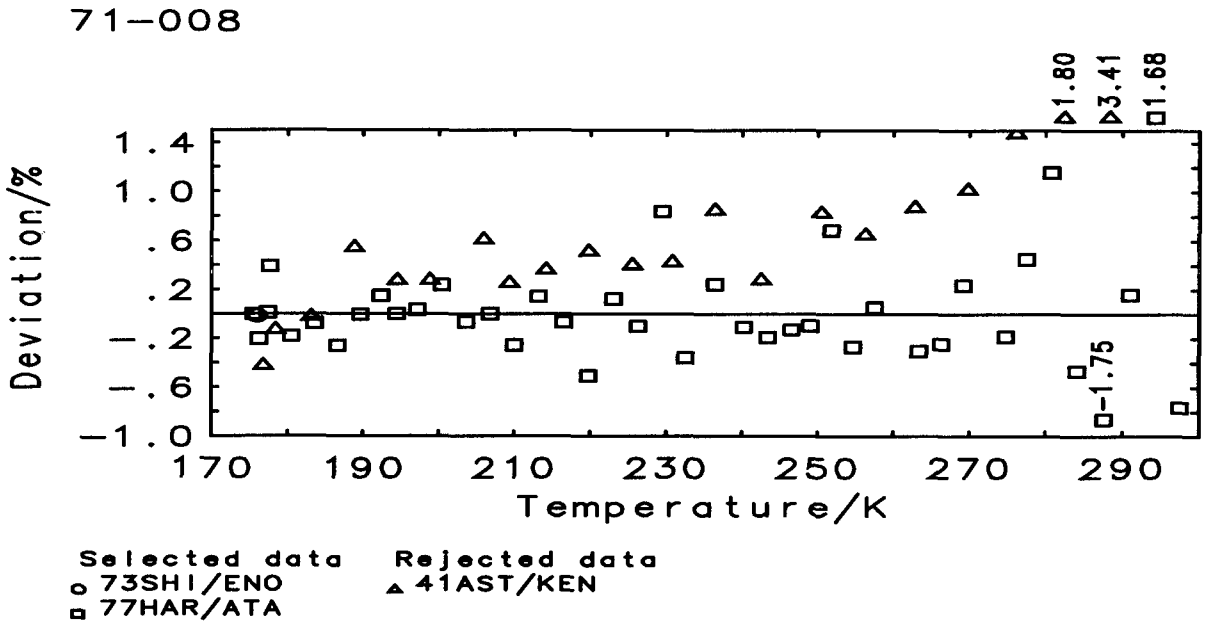
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	68	46	1.013	1.14–1	0.51	–1.47–3	–6
Temp. range K		A_1	A_2	A_3			Level of uncertainty
175.5–297.5		1.65216+1	1.26555	3.21600–1			III

TABLE 71.8.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.870	1.893	1.917	1.941	1.966	1.992	2.018
C_p (J K^{-1}mol^{-1})	165.0	167.0	169.1	171.3	173.5	175.7	178.0
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	2.045	2.072	2.100	2.109	2.129	2.158	2.182
C_p (J K^{-1}mol^{-1})	180.4	182.8	185.3	186.1	187.8	190.4	192.5
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	2.188						
C_p (J K^{-1}mol^{-1})	193.0						

TABLE 71.8.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	68	46	1.020	1.13–1	0.51	1.15–3	–4
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
175.5–297.5	448.64	–2.02985	1.37393–1	1.55524+1	7.49731		III



Name: 1,1–Dimethylsilacyclobutane
Formula: $C_5H_{12}Si$

CAS–RN: 2295–12–7
Group No.: 71–009
Molar Mass: 100.24

TABLE 71.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73GUS/DZH	155.4–298.1	6S	nosp	99.63	melpt	C_p	BSAO	54STR/ICK

TABLE 71.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.371	3.78–2	0.19	5.18–5	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
155.4–298.1		1.97387+1	–1.80423	1.05763			III

TABLE 71.9.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.622	1.636	1.652	1.670	1.689	1.710	1.733
C_p (J K^{-1}mol^{-1})	162.6	164.0	165.6	167.4	169.3	171.4	173.7
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.757	1.783	1.811	1.841	1.873	1.883	1.906
C_p (J K^{-1}mol^{-1})	176.1	178.8	181.6	184.6	187.7	188.8	191.1
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	1.941	1.971	1.978				
C_p (J K^{-1}mol^{-1})	194.6	197.6	198.3				

Name: Ethenyltrimethylsilane
Formula: $C_5H_{12}Si$

CAS–RN: 754–05–2
Group No.: 71–010
Molar Mass: 100.24

TABLE 71.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73LEB/TSV	141.6–300.0	6S	0.50	99.67	melpt	C_p	BSAO	66NIK/LEB

TABLE 71.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	1.025	1.11–1	0.51	5.93–4	0
Temp. range K		A_1	A_2				Level of uncertainty
141.6–300.0		1.76188+1	2.11164				III

TABLE 71.10.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.724	1.742	1.759	1.777	1.794	1.812	1.829
C_p (J K^{-1}mol^{-1})	172.8	174.6	176.3	178.1	179.9	181.6	183.4
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.847	1.864	1.882	1.899	1.917	1.934	1.940
C_p (J K^{-1}mol^{-1})	185.1	186.9	188.6	190.4	192.1	193.9	194.4
Temp. (K)	280	290	298.15	300			
c_p (J K^{-1}g^{-1})	1.952	1.969	1.984	1.987			
C_p (J K^{-1}mol^{-1})	195.7	197.4	198.8	199.2			

Name: Trichlorophenylsilane
Formula: $C_6H_5Cl_3Si$

CAS–RN: 98–13–5
Group No.: 71–011
Molar Mass: 211.55

TABLE 71.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65GUM/KOS1	247.2–288.6	19	nosp	99.49	melpt	C_p	BSAO	54STR/ICK

TABLE 71.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.709	2.71–1	1.06	5.18–3	–1

Temp. range K	A_1	A_2	Level of uncertainty
247.2–288.6	1.84730+1	2.63944	V

TABLE 71.11.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p ($J K^{-1} g^{-1}$)	0.99	1.00	1.01	1.01	1.02	1.03	1.04
C_p ($J K^{-1} mol^{-1}$)	208	211	213	214	215	217	219

Name: Chlorotriethylsilane
Formula: $C_6H_{15}ClSi$

CAS–RN: 994–30–9
Group No.: 71–012
Molar Mass: 150.72

TABLE 71.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69NAG/DZH2	197.1–298.1	12S	nosp	98.24	melpt	C_p	BSAO	54STR/ICK

TABLE 71.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.153	2.32–2	0.08	2.57–5	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
197.1–298.1	1.70807+1	6.74073	–5.95541–1	V

TABLE 71.12.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1} g^{-1}$)	1.55	1.58	1.60	1.62	1.65	1.67	1.69
C_p ($J K^{-1} mol^{-1}$)	234	238	241	245	248	251	254
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J K^{-1} g^{-1}$)	1.71	1.71	1.73	1.74	1.76	1.76	
C_p ($J K^{-1} mol^{-1}$)	257	258	260	263	265	266	

Name: 1,1,3,3–Tetramethyl–1,3–disilacyclobutane
Formula: $C_6H_{16}Si_2$

CAS–RN: 1627–98–1
Group No.: 71–013
Molar Mass: 144.36

TABLE 71.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73DZH/GUS	266.0–298.1	3S	nosp	99.96	melpt	C_p	BSAO	54STR/ICK

TABLE 71.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.041	5.19–3	0.02	6.36–7	–1
Temp. range K		A_1	A_2				Level of uncertainty
266.0–298.1		1.79245+1	2.73867				IV

TABLE 71.13.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.458	1.463	1.474	1.490	1.503	1.506
C_p ($J K^{-1} mol^{-1}$)	210.5	211.2	212.8	215.1	216.9	217.3

Name: Hexamethyldisiloxane
Formula: $C_6H_{18}OSi_2$

CAS–RN: 107–46–0
Group No.: 71–014
Molar Mass: 162.38

TABLE 71.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
61SCO/MES	208.9–370.9	20	0.20	99.996	melpt	C_{sat}	BSAO	47HUF
75PED/KAY	301.5–345.8	8	nosp	not specified		C_p	BSIO	75PED/KAY
86DZH/KUL	204.0–375.0	eqn	0.20	99.9	melpt	C_p	BSAO	54STR/ICK

TABLE 71.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
61SCO/MES	208.9–370.9	20	0.20	0.285	2.19–2	0.06	–2.40–3	–1
75PED/KAY	301.5–345.8	8	0.40#	0.905	1.42–1	0.36	2.52–2	2
				Rejected data				
86DZH/KUL	(6.95, 14.90, 6.38, 8)							

TABLE 71.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	38	28	0.572	8.26–2	0.21	5.48–3	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
208.9–370.9		2.75893+1	1.84052	4.90558–1			II

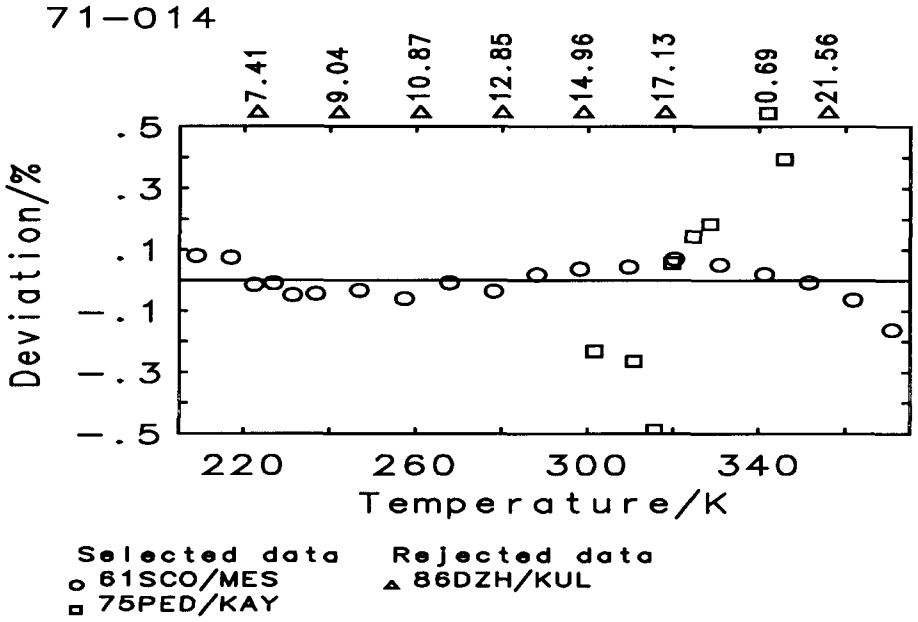
TABLE 71.14.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c ($J K^{-1} g^{-1}$)	1.721	1.742	1.762	1.784	1.805	1.828	1.850
C ($J K^{-1} mol^{-1}$)	279.5	282.8	286.2	289.6	293.1	296.8	300.4
Temp. (K)	273.15	280	290	298.15	300	310	320
c ($J K^{-1} g^{-1}$)	1.858	1.873	1.897	1.917	1.921	1.946	1.971
C ($J K^{-1} mol^{-1}$)	301.6	304.2	308.1	311.3	312.0	316.0	320.1
Temp. (K)	330	340	350	360	370		
c ($J K^{-1} g^{-1}$)	1.997	2.023	2.050	2.077	2.105		
C ($J K^{-1} mol^{-1}$)	324.3	328.6	332.9	337.3	341.9		

TABLE 71.14.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	38	28	0.766	8.98–2	0.23	5.86–3	1

Temp. range K	T_c K	A_1	A_2	A_3	A_4	Level of uncertainty
208.9–370.9	518.70	–4.19399	3.44899–1	2.56906+1	1.27498+1	II



Name: Hexamethylcyclotrisiloxane
Formula: $C_6H_{18}O_3Si_3$

CAS-RN: 541-05-9
Group No.: 71-015
Molar Mass: 222.46

TABLE 71.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
77KUL/DZH2	335.2–350.0	3S	nosp	not specified		C_p	BSAO	54STR/ICK

TABLE 71.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.059	2.82–2	0.06	1.40–5	1
Temp. range K		A_1	A_2				Level of uncertainty
335.2–350.0		2.02759+1	8.05180				V

TABLE 71.15.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p ($J K^{-1} g^{-1}$)	1.78	1.81
C_p ($J K^{-1} mol^{-1}$)	396	403

Name: Hexamethyldisilane
Formula: $C_6H_{18}Si_2$

CAS–RN: 1450–14–2
Group No.: 71–016
Molar Mass: 146.38

TABLE 71.16.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
59SUG/SEK	N	289.9–295.7	5	nosp	99.87	melpt	C_p	BDHO	55SEK/MOM

59SUG/SEK C_p at the highest temperature was misprinted, correct value 61.66 cal/(K.mol)

TABLE 71.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	1.061	2.28–1	0.74	2.03–3	–1
Temp. range K		A_1	A_2				Level of uncertainty
289.9–295.7		4.26158	9.04807				IV

TABLE 71.16.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300
c_p (J K^{-1}g^{-1})	1.732	1.774	1.784
C_p (J K^{-1}mol^{-1})	253.6	259.7	261.1

Name: 2,2,4,4,6,6–Hexamethylcyclotrisilazane
Formula: $C_6H_{21}N_3Si_3$

CAS–RN: 1009–93–4
Group No.: 71–017
Molar Mass: 219.51

TABLE 71.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67NAG/KAR2	255.4–298.1	10S	nosp	99.2	melpt	C_p	BSAO	54STR/ICK

TABLE 71.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.092	4.58–2	0.09	7.67–5	–2
Temp. range K		A_1	A_2				Level of uncertainty
255.4–298.1		2.52793+1	8.75579				V

TABLE 71.17.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.82	1.85	1.86	1.89	1.92	1.95	1.95
C_p (J K^{-1}mol^{-1})	399	407	409	414	421	427	429

Name: Dichloromethylphenylsilane
Formula: $C_7H_8Cl_2Si$

CAS-RN: 149-74-6
Group No.: 71-018
Molar Mass: 191.13

TABLE 71.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
65GUM/KOS3	234.8–297.4	25	nosp	99.41	melpt	C_p	BSAO	54STR/ICK

TABLE 71.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	25	25	1.055	5.92-1	2.11	2.27-2	-4
Temp. range K		A_1	A_2				Level of uncertainty
234.8–297.4		1.57058+1	4.98252				V

TABLE 71.18.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.18	1.20	1.23	1.25	1.27	1.28	1.29
C_p ($J K^{-1}mol^{-1}$)	226	230	234	238	242	244	247
Temp. (K)	290	298.15	300				
c_p ($J K^{-1}g^{-1}$)	1.31	1.33	1.33				
C_p ($J K^{-1}mol^{-1}$)	251	254	255				

Name: Methylenebis[trimethylsilane]
Formula: $C_7H_{20}Si_2$

CAS-RN: 2117-28-4
Group No.: 71-019
Molar Mass: 160.41

TABLE 71.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82GUS/KAR	140.6–300.0	19S	0.30	99.05	melpt	C_p	BSAO	54STR/ICK

TABLE 71.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	19	19	0.055	6.30-3	0.02	8.03-7	-1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
140.6–300.0		2.24417+1	7.09823	-6.93548-2			V

TABLE 71.19.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.71	1.74	1.78	1.81	1.85	1.88	1.92
C_p (J K^{-1}mol^{-1})	274	280	285	291	297	302	308
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.96	1.99	2.03	2.06	2.10	2.13	2.14
C_p (J K^{-1}mol^{-1})	314	319	325	331	336	342	343
Temp. (K)	280	290	298.15	300			
c_p (J K^{-1}g^{-1})	2.17	2.20	2.23	2.23			
C_p (J K^{-1}mol^{-1})	347	353	357	358			

Name: 1-[2-(Trimethylsilyl)ethyl]azetidine
Formula: $C_8H_{19}NSi$

CAS-RN: 42525-64-4
Group No.: 71-020
Molar Mass: 157.33

TABLE 71.20.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77LEB/RAB1	N	202.6–304.6	33	0.30	99.345	melpt	C_p	BSAO	66NIK/LEB

77LEB/RAB1 same data in 75LEB/RAB

TABLE 71.20.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	33	33	0.567	5.86-2	0.17	1.79-4	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
202.6–304.6		2.63959+1	2.47241-1	1.06586			III

TABLE 71.20.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.646	1.671	1.696	1.723	1.751	1.780	1.810
C_p (J K^{-1}mol^{-1})	259.0	262.9	266.9	271.1	275.4	280.0	284.7
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	1.841	1.851	1.873	1.907	1.935	1.941	
C_p (J K^{-1}mol^{-1})	289.6	291.2	294.7	300.0	304.4	305.4	

Name: Tetraethyl ester silicic acid
Formula: $C_8H_{20}O_4Si$

CAS–RN: 78–10–4
Group No.: 71–021
Molar Mass: 208.33

TABLE 71.21.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
*80OGI	N	329.6	1	nosp	not specified	C_{sng}	DSIO	*79BER
85NKI/CHA		298.0	1	0.30	not specified	C_p	FSIT	71PIC/LED
92VAN/COR		193.6–361.3	94	0.15	not specified	C_p	BSAO	87VAN/VAN

*80OGI average value in temperature range 288–371 K

TABLE 71.21.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
92VAN/COR	193.6–361.3	92	0.15	0.279	1.80–2	0.04	1.44–5	0
				Rejected data				
*80OGI	(8.33–1, 1.86,–8.33–1, –1)			85NKI/CHA	(1.44, 3.40,–1.44, –1)			

TABLE 71.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	96	92	0.285	1.84–2	0.04	1.44–5	0
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
193.6–361.3	5.02522+1	–1.31763+1	4.91203	–4.08966–1			III

TABLE 71.21.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J\,K^{-1}g^{-1}$)	1.607	1.615	1.624	1.635	1.647	1.661	1.677
C_p ($J\,K^{-1}mol^{-1}$)	334.9	336.4	338.3	340.5	343.1	346.1	349.3
Temp. (K)	270	273.15	280	290	298.15	300	310
c_p ($J\,K^{-1}g^{-1}$)	1.694	1.699	1.712	1.731	1.748	1.752	1.773
C_p ($J\,K^{-1}mol^{-1}$)	352.8	354.0	356.6	360.7	364.1	364.9	369.4
Temp. (K)	320	330	340	350	360		
c_p ($J\,K^{-1}g^{-1}$)	1.795	1.819	1.842	1.867	1.892		
C_p ($J\,K^{-1}mol^{-1}$)	374.0	378.9	383.8	388.9	394.1		

TABLE 71.21.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	96	92	1.321	8.41–2	0.20	3.05–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
193.6–361.3	575.90	5.39471–1	6.82068	2.99452+1	1.06671–2		III

Name: Tetraethylsilane
Formula: $C_8H_{20}Si$

CAS–RN: 631–36–7
Group No.: 71–022
Molar Mass: 144.33

TABLE 71.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
54STA/WAR	190.0–220.0	4S	1.00	99.9	melpt	C_p	BSAO	49STA/GUP
72MAS/RAB	200.0–300.0	12S	0.40	99.8	melpt	C_p	BSAO	56POP/KOL

TABLE 71.22.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
72MAS/RAB	200.0–300.0	12	0.40	0.088	1.17–2	0.04	7.95–6	–3
				Rejected data				
54STA/WAR	(3.53–1, 1.10, 3.31–1, 3)							

TABLE 71.22.3. Parameters of regression polynomial

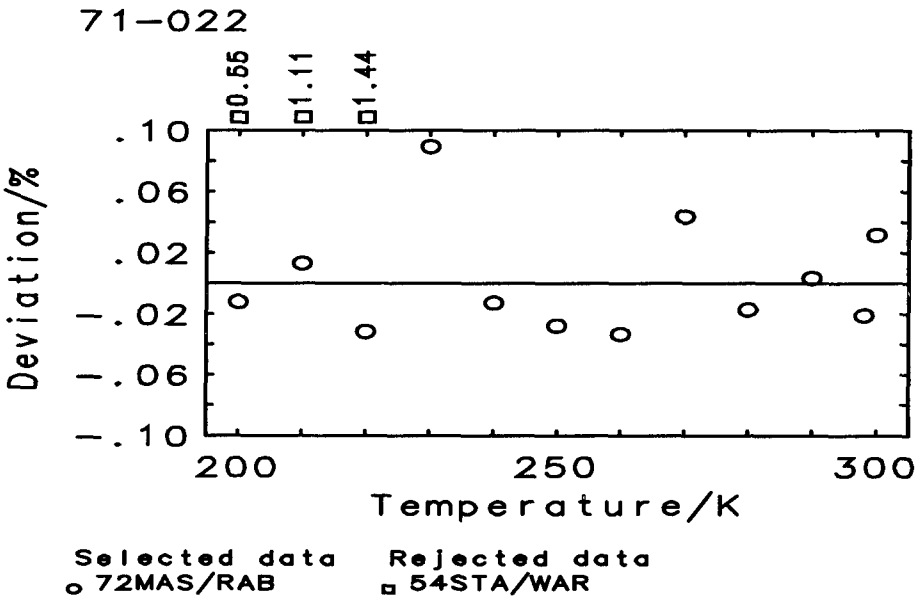
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	16	12	0.102	1.35–2	0.04	7.95–6	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
200.0–300.0		2.85299+1	–8.35423–1	1.10508			III

TABLE 71.22.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1} g^{-1}$)	1.802	1.823	1.846	1.870	1.895	1.921	1.949
C_p ($J K^{-1} mol^{-1}$)	260.1	263.1	266.4	269.8	273.5	277.3	281.3
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J K^{-1} g^{-1}$)	1.978	1.987	2.008	2.039	2.066	2.072	
C_p ($J K^{-1} mol^{-1}$)	285.4	286.8	289.8	294.3	298.2	299.1	

TABLE 71.22.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	12	0.106	1.42–2	0.04	7.31–6	–1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
200.0–300.0	603.70	–4.78265	6.50268	1.93289+1	8.79396–1		III



Name: Octamethylcyclotetrasiloxane
Formula: $C_8H_{24}O_4Si_4$

CAS–RN: 556–67–2
Group No.: 71–023
Molar Mass: 296.62

TABLE 71.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
75MEK/KAR1	290.5–310.0	4S	nosp	not specified	C_p	BSAO	54STR/ICK

TABLE 71.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.033	1.33–2	0.03	9.54–6	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
290.5–310.0		–7.44495+2	5.08756+2	–8.23138+1			V

TABLE 71.23.4. Recommended values of heat capacities

Temp. (K)	295	298.15	300	305	310
c_p (J K^{-1}g^{-1})	1.12	1.14	1.15	1.16	1.17
C_p (J K^{-1}mol^{-1})	333	338	340	345	346

Name: 2,2,4,4,6,6,8,8–Octamethylcyclotetrasilazane
Formula: $C_8H_{28}N_4Si_4$

CAS–RN: 1020–84–4
Group No.: 71–024
Molar Mass: 292.68

TABLE 71.24.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67NAG/KAR1	370.0–385.0	4S	nosp	99.03	melpt	C_p	BSAO	54STR/ICK

TABLE 71.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.124	8.20–2	0.12	1.03–4	0

Temp. range K	A_1	A_2	Level of uncertainty
370.0–385.0	–4.33457+1	2.90165+1	V

TABLE 71.24.4. Recommended values of heat capacities

Temp. (K)	370	380	390
c_p (J K^{-1}g^{-1})	1.82	1.90	1.98
C_p (J K^{-1}mol^{-1})	532	556	581

Name: (3–Chloropropyl)triethoxysilane
Formula: $C_9H_{21}ClO_3Si$

CAS–RN: 5089–70–3
Group No.: 71–025
Molar Mass: 240.80

TABLE 71.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
67KAR/MEK	135.0–300.0	34S	nosp	not specified		C_p	BSAO	54STR/ICK

TABLE 71.25.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	34	34	0.577	2.32–1	0.46	1.90–3	2

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
135.0–300.0	3.30730+1	2.56011+1	–1.30165+1	2.17092	V

TABLE 71.25.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p (J K^{-1}g^{-1})	1.70	1.71	1.71	1.71	1.71	1.71	1.71
C_p (J K^{-1}mol^{-1})	410	412	412	413	413	413	412
Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.71	1.71	1.71	1.71	1.71	1.72	1.73
C_p (J K^{-1}mol^{-1})	412	412	412	412	413	414	416
Temp. (K)	273.15	280	290	298.15	300		
c_p (J K^{-1}g^{-1})	1.73	1.74	1.75	1.77	1.77		
C_p (J K^{-1}mol^{-1})	417	419	422	426	427		

Name: 3-(Triethoxysilyl)-1-propanamine
Formula: $C_9H_{23}NO_3Si$

CAS-RN: 919-30-2
Group No.: 71-026
Molar Mass: 221.37

TABLE 71.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
67KAR/MEK	145.0–300.0	32S	nosp	not specified	C_p	BSAO	54STR/ICK

TABLE 71.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	32	32	0.099	5.13-2	0.10	9.17-5	–4
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
145.0–300.0		6.42136+1	–2.18455+1	1.04551+1	–1.39289		V

TABLE 71.26.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	1.89	1.89	1.89	1.90	1.91	1.92	1.94
C_p (J K^{-1}mol^{-1})	418	418	419	421	423	426	429
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.95	1.97	1.98	2.00	2.01	2.03	2.03
C_p (J K^{-1}mol^{-1})	432	435	439	442	446	449	450
Temp. (K)	280	290	298.15	300			
c_p (J K^{-1}g^{-1})	2.04	2.06	2.07	2.07			
C_p (J K^{-1}mol^{-1})	453	456	458	459			

Name: 1,3–Propanediylbis[trimethylsilane]
Formula: $C_9H_{24}Si_2$

CAS–RN: 2295–05–8
Group No.: 71–027
Molar Mass: 188.46

TABLE 71.27.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75GUS/KAR	N	225.7–300.0	37	nosp	98.23	melpt	C_p	BSAO	54STR/ICK

75GUS/KAR only a graph given in the paper; experimental values provided by the authors

TABLE 71.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	37	37	0.154	6.92–2	0.15	1.97–4	–2

Temp. range K	A_1	A_2	A_3	Level of uncertainty
225.7–300.0	2.53220+1	9.03687	–5.41161–1	V

TABLE 71.27.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1}g^{-1}$)	1.91	1.94	1.96	1.99	2.02	2.03	2.05
C_p ($J K^{-1}mol^{-1}$)	360	365	370	375	381	382	386

Temp. (K)	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	2.07	2.09	2.10
C_p ($J K^{-1}mol^{-1}$)	391	395	395

Name: 1,1,3,3,5,5–Hexamethyl–1,3,5–trisilacyclohexane
Formula: $C_9H_{24}Si_3$

CAS–RN: 1627–99–2
Group No.: 71–028
Molar Mass: 216.55

TABLE 71.28.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75GUS/DZH	268.6–300.0	7S	0.30	98.14	melpt	C_p	BSAO	54STR/ICK

TABLE 71.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.111	1.60–2	0.03	7.63–6	1

Temp. range K	A_1	A_2	Level of uncertainty
268.6–300.0	3.43927+1	4.64885	V

TABLE 71.28.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.80	1.81	1.82	1.84	1.85	1.86
C_p ($J K^{-1}mol^{-1}$)	390	392	394	398	401	402

Name: Ethenyldimethylphenylsilane
Formula: $C_{10}H_{14}Si$

CAS–RN: 1125–26–4
Group No.: 71–029
Molar Mass: 162.31

TABLE 71.29.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74LEB/ARO	N	190.7–300.0	5S	0.50	99.14	melpt	C_p	BSAO	66NIK/LEB

74LEB/ARO same data in 77LEB/RAB2

TABLE 71.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.140	2.10–2	0.07	1.07–5	1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
190.7–300.0	2.45663+1	1.53541	5.75448–1	IV

TABLE 71.29.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	1.534	1.554	1.574	1.595	1.617	1.639	1.662
C_p ($J K^{-1}mol^{-1}$)	248.9	252.2	255.5	258.9	262.5	266.1	269.8

Temp. (K)	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.686	1.693	1.710	1.734	1.755	1.760
C_p ($J K^{-1}mol^{-1}$)	273.6	274.8	277.5	281.5	284.9	285.6

Name: 2,2,4,4–Tetraethyl–6,6–dimethylcyclotrisiloxane
Formula: $C_{10}H_{26}O_3Si_3$

CAS–RN: 110505–51–6
Group No.: 71–030
Molar Mass: 278.57

TABLE 71.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
87DZH/KUL3	N	261.3–299.9	13	nosp	99.	chrom	C_p	BSAO	54STR/ICK

87DZH/KUL3 two samples of different purity; results with low purity were omitted

TABLE 71.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.948	5.54–1	0.95	8.93–3	1
Temp. range K		A_1	A_2				Level of uncertainty
261.3–299.9		3.52731+1	8.33939				V

TABLE 71.30.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.70	1.72	1.73	1.75	1.77	1.79	1.80
C_p (J K^{-1}mol^{-1})	474	480	483	487	494	500	501

Name: Ethenyldimethyl(phenylmethyl)silane
Formula: $C_{11}H_{16}Si$

CAS–RN: 18001–46–2
Group No.: 71–031
Molar Mass: 176.33

TABLE 71.31.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
79LEB/LEB2	204.0–320.0	4S	0.20	99.37	melpt	C_p	BSAO	76LEB/LIT

TABLE 71.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	8.723	6.68–1	1.75	1.19–2	2
Temp. range K		A_1	A_2				Level of uncertainty
204.0–320.0		2.73335+1	3.66985				V

TABLE 71.31.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p (J K^{-1}g^{-1})	1.65	1.67	1.69	1.70	1.72	1.74	1.76
C_p (J K^{-1}mol^{-1})	291	294	297	300	304	307	310
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.76	1.77	1.79	1.80	1.81	1.83	1.84
C_p (J K^{-1}mol^{-1})	311	313	316	318	319	322	325

Name: [1,1'–Biphenyl]–2–yltrichlorosilane
Formula: $C_{12}H_9Cl_3Si$

CAS–RN: 18030–62–1
Group No.: 71–032
Molar Mass: 287.65

TABLE 71.32.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74GEI/DZH1	N	338.0–370.0	3S	nosp	not specified		C_p	BSAO	54STR/ICK

74GEI/DZH1 low purity of sample

TABLE 71.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.037	5.54–2	0.11	3.94–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
338.0–370.0		3.28024+1	4.73963				VI

TABLE 71.32.4. Recommended values of heat capacities

Temp. (K)	340	350	360	370
c_p ($J K^{-1} g^{-1}$)	1.41	1.43	1.44	1.46
C_p ($J K^{-1} mol^{-1}$)	407	411	415	419

Name: [1,1'–Biphenyl]–4–yltrichlorosilane
Formula: $C_{12}H_9Cl_3Si$

CAS–RN: 18030–61–0
Group No.: 71–033
Molar Mass: 287.65

TABLE 71.33.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76GEI/DZH	371.9–380.0	2S	nosp	98.4	melpt	C_p	BSAO	54STR/ICK

TABLE 71.33.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
371.9–380.0		1.58117+1	8.01811				VI

TABLE 71.33.4. Recommended values of heat capacities

Temp. (K)	375	380
c_p ($J K^{-1} g^{-1}$)	1.33	1.34
C_p ($J K^{-1} mol^{-1}$)	381	385

Name: Tetrapropyl ester silicic acid
Formula: $C_{12}H_{28}O_4Si$

CAS-RN: 682-01-9
Group No.: 71-034
Molar Mass: 264.44

TABLE 71.34.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
85NKI/CHA	298.00	1.740	0.30	not specified		C_p	FSIT	71PIC/LED

Name: Hexaethyldisiloxane
Formula: $C_{12}H_{30}OSi_2$

CAS-RN: 994-49-0
Group No.: 71-035
Molar Mass: 246.54

TABLE 71.35.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86DZH/KUL	200.0-300.0	eqn	0.20	97.	melpt	C_p	BSAO	54STR/ICK

TABLE 71.35.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	10	10	0.000	2.50-6	0.00	1.14-6	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
200.0-299.9	3.39431+1	7.52896	-1.26277-1	V

TABLE 71.35.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1}g^{-1}$)	1.64	1.66	1.68	1.71	1.73	1.75	1.78
C_p ($J K^{-1}mol^{-1}$)	403	409	415	421	426	432	438
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J K^{-1}g^{-1}$)	1.80	1.81	1.82	1.85	1.86	1.87	
C_p ($J K^{-1}mol^{-1}$)	444	445	449	455	460	461	

Name: Hexaethylcyclotrisiloxane
Formula: $C_{12}H_{30}O_3Si_3$

CAS-RN: 2031-79-0
Group No.: 71-036
Molar Mass: 306.62

TABLE 71.36.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82KUL/LEB2	N	292.5-329.7	12	0.20	99.7	melpt	C_p	BSAO	76LEB/LIT
85DZH/KUL		280.2-300.0	4S	0.30	96.5	melpt	C_p	BSAO	54STR/ICK

82KUL/LEB2 same data in 82KUL/LEB1, 88LEB/KUL and smoothed value in 84LEB/KUL

TABLE 71.36.2. Correlated heat capacities

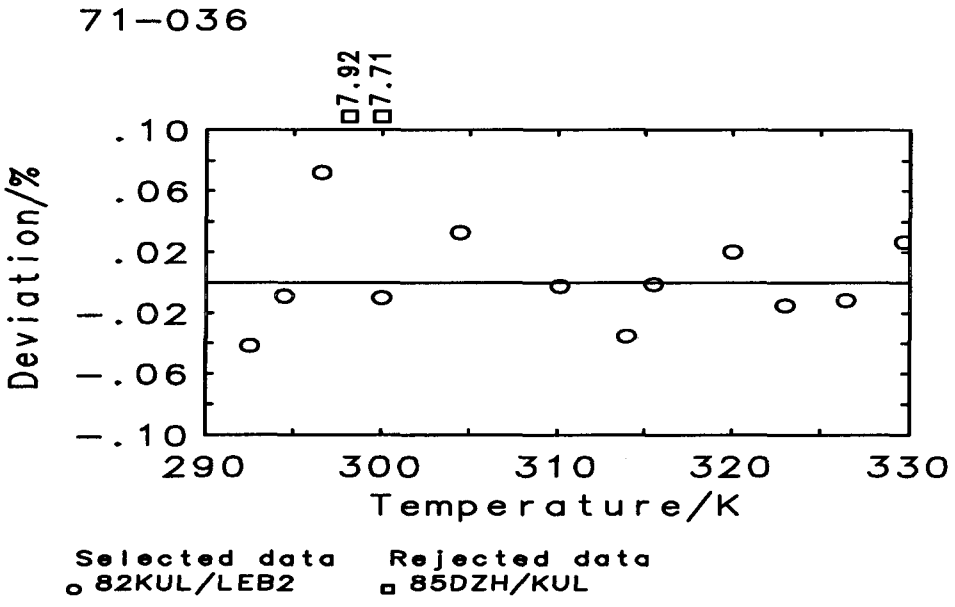
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
82KUL/LEB2	292.5–329.7	12	0.20	0.150	1.95–2	0.03	1.11–5	–2
				Rejected data				
85DZH/KUL	(5.47, 7.82, 5.47, 2)							

TABLE 71.36.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	16	12	0.174	2.25–2	0.03	1.11–5	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
292.5–329.7		6.07949+1	–5.43375	2.22657			III

TABLE 71.36.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330
c_p ($J K^{-1} g^{-1}$)	1.729	1.746	1.750	1.772	1.795	1.820
C_p ($J K^{-1} mol^{-1}$)	530.2	535.3	536.6	543.3	550.5	558.0



Name: 1,1,1,3,5,5,5–Heptamethyl–3–phenyltrisiloxane
Formula: $C_{13}H_{26}O_2Si_3$

CAS–RN: 546–44–1
Group No.: 71–037
Molar Mass: 298.60

TABLE 71.37.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84DZH/KUL	226.8–300.0	10S	0.30	97.4	melpt	C_p	BSAO	54STR/ICK

TABLE 71.37.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.166	2.80–2	0.05	1.18–5	–1

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
226.8–300.0	1.33763+2	–9.97778+1	3.82399+1	–4.29077	VI

Table 71.37.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p ($J K^{-1} g^{-1}$)	1.51	1.54	1.57	1.60	1.63	1.65	1.67
C_p ($J K^{-1} mol^{-1}$)	452	459	468	477	488	491	499

Temp. (K)	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.71	1.74	1.75
C_p ($J K^{-1} mol^{-1}$)	510	520	522

Name: Diethynyldiphenylsilane
Formula: $C_{16}H_{12}Si$

CAS–RN: 1675–57–6
Group No.: 71–038
Molar Mass: 232.36

TABLE 71.38.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74MIL/LEB		316.2–330.0	3S	0.50	99.04	melpt	C_p	BSAO	66NIK/LEB
77MIL/LEB	N	318.3–325.7	11	0.20	not specified		C_p	BSAO	76LEB/LIT

77MIL/LEB completion of data published by 74MIL/LEB

TABLE 71.38.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74MIL/LEB	316.2–330.0	3	0.50	1.716	4.15–1	0.86	3.15–1	1
77MIL/LEB	318.5–325.7	10	0.20	0.870	8.28–2	0.17	–1.44–2	0

TABLE 71.38.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	14	13	1.281	2.42–1	0.50	6.15–2	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
316.2–330.0		1.49054+3	–9.03411+2	1.41385+2			IV

TABLE 71.38.4. Recommended values of heat capacities

Temp. (K)	320	330
c_p ($J K^{-1} g^{-1}$)	1.696	1.752
C_p ($J K^{-1} mol^{-1}$)	394.2	407.2

Name: 1,1,3,3–Tetramethyl–1,3–diphenyldisiloxane
Formula: $C_{16}H_{22}OSi_2$

CAS–RN: 56–33–7
Group No.: 71–039
Molar Mass: 286.52

TABLE 71.39.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Reference
83DZH/KUL		250.0–300.0	7S	0.20	not specified	C_p	BSAO	54STR/ICK
86DZH/KUL	N	170.0–300.0	eqn	0.20	not specified	C_p	BSAO	54STR/ICK

86DZH/KUL low temperature limit is below n.m.t.; undercooled liquid

TABLE 71.39.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
83DZH/KUL	250.0–300.0	7	0.20	0.849	1.00–1	0.17	2.62–2	2
86DZH/KUL	170.0–299.6	13	0.20	0.529	6.21–2	0.11	–1.38–2	1

TABLE 71.39.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	20	20	0.715	8.42–2	0.14	2.21–4	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
170.0–300.0		4.75588+1	–1.94992	2.15940			V

TABLE 71.39.4. Recommended values of heat capacities

Temp. (K)	170	180	190	200	210	220	230
c_p (J K^{-1}g^{-1})	1.47	1.48	1.50	1.52	1.54	1.56	1.58
C_p (J K^{-1}mol^{-1})	420	424	429	435	441	447	453
Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.61	1.63	1.66	1.68	1.69	1.71	1.74
C_p (J K^{-1}mol^{-1})	460	467	475	483	485	491	499
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.77	1.77					
C_p (J K^{-1}mol^{-1})	507	508					

Name: 2,2,4,4–Tetramethyl–6,6–diphenylcyclotrisiloxane
Formula: $C_{16}H_{22}O_3Si_3$

CAS–RN: 1693–51–2
Group No.: 71–040
Molar Mass: 346.61

TABLE 71.40.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
82KUL/DZH N	340.3–351.4	5	0.20	97.06 melpt	C_p	BSAO	54STR/ICK

82KUL/DZH only a graph given in the paper; experimental values provided by the authors

TABLE 71.40.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.471	6.76–2	0.09	7.48–5	1
Temp. range K		A_1	A_2				Level of uncertainty
340.3–351.4		3.91583+1	9.49578				V

TABLE 71.40.4. Recommended values of heat capacities

Temp. (K)	340	350
c_p (J K^{-1}g^{-1})	1.71	1.74
C_p (J K^{-1}mol^{-1})	594	602

Name: Tetrabutyl ester silicic acid
Formula: $C_{16}H_{36}O_4Si$

CAS–RN: 4766–57–8
Group No.: 71–041
Molar Mass: 320.54

TABLE 71.41.1. Experimental heat capacities

Reference	Temp. K	Capac. J/(K.g)	Error %	Purity % method	Type capacity	Calorimeter Type	Calorimeter Reference
85NKI/CHA	298.00	1.810	0.30	not specified	C_p	FSIT	71PIC/LED

Name: Octaethylcyclotetrasiloxane
Formula: $C_{16}H_{40}O_4Si_4$

CAS-RN: 1451-99-6
Group No.: 71-042
Molar Mass: 408.83

TABLE 71.42.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87DZH/KUL1	212.9–300.0	11S	0.50	98.4	melpt	C_p	BSAO	54STR/ICK

TABLE 71.42.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	11	11	0.198	8.09-2	0.10	4.02-5	-1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
212.9–300.0		3.93178+2	-3.71085+2	1.41926+2	-1.73051+1		V

TABLE 71.42.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J K^{-1} g^{-1}$)	1.62	1.63	1.64	1.67	1.70	1.73	1.74
C_p ($J K^{-1} mol^{-1}$)	661	664	672	683	695	709	713
Temp. (K)	280	290	298.15	300			
c_p ($J K^{-1} g^{-1}$)	1.77	1.80	1.83	1.83			
C_p ($J K^{-1} mol^{-1}$)	723	736	746	748			

Name: 1-[2-(Trimethylsilyl)ethyl]aziridine
Formula: $C_{17}H_{17}NSi$

CAS-RN: 18387-12-7
Group No.: 71-043
Molar Mass: 263.41

TABLE 71.43.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
74LEB/TSV	182.8–299.5	21	0.50	98.93	melpt	C_p	BSAO	66NIK/LEB

TABLE 71.43.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	21	21	0.378	6.35-2	0.19	1.95-4	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
182.9–299.5		3.21177+1	-4.08927	1.81095			IV

TABLE 71.43.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	0.967	0.975	0.984	0.995	1.006	1.019	1.033
C_p (J K^{-1}mol^{-1})	254.6	256.8	259.3	262.0	265.1	268.5	272.2
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.048	1.065	1.082	1.088	1.101	1.120	1.137
C_p (J K^{-1}mol^{-1})	276.1	280.4	285.0	286.5	289.9	295.1	299.5
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.141						
C_p (J K^{-1}mol^{-1})	300.6						

Name: Chlorotriphenylsilane
Formula: $C_{18}H_{15}ClSi$

CAS–RN: 76–86–8
Group No.: 71–044
Molar Mass: 294.86

TABLE 71.44.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
68KOS/MOS	379.0–386.9	3	nosp	98.59	melpt	C_p	BSAO	54STR/ICK

TABLE 71.44.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.163	9.60–2	0.16	1.04–4	1
Temp. range K		A_1	A_2				Level of uncertainty
379.0–386.9		1.74567+1	1.07114+1				V

TABLE 71.44.4. Recommended values of heat capacities

Temp. (K)	380	390
c_p (J K^{-1}g^{-1})	1.64	1.67
C_p (J K^{-1}mol^{-1})	484	492

Name: 1,1,1,5,5,5–Hexamethyl–3,3–diphenyltrisiloxane
Formula: $C_{18}H_{28}O_2Si_3$

CAS–RN: 797–77–3
Group No.: 71–045
Molar Mass: 360.68

TABLE 71.45.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
81SHA/DZH	N	271.0–298.0	2S	0.30	99.41	melpt	C_p	BSAO	54STR/ICK

81SHA/DZH data point at 271 K taken from a graph

TABLE 71.45.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
271.0–298.0		5.13872+1	8.90901				IV

TABLE 71.45.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.760	1.780	1.797	1.801
C_p ($J K^{-1}mol^{-1}$)	634.7	642.1	648.1	649.5

Name: 2,2,4,4,6,6–Hexamethyl–8,8–diphenylcyclotetrasiloxane
Formula: $C_{18}H_{28}O_4Si_4$

CAS–RN: 30026–85–8
Group No.: 71–046
Molar Mass: 420.76

TABLE 71.46.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75MEK/KAR2	305.1–320.0	3S	0.30	99.28	melpt	C_p	BSAO	54STR/ICK

TABLE 71.46.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.108	2.58–2	0.03	–1.78–5	0
Temp. range K		A_1	A_2				Level of uncertainty
305.1–320.0		–8.66581+1	5.36278+1				IV

TABLE 71.46.4. Recommended values of heat capacities

Temp. (K)	310	320
c_p ($J K^{-1}g^{-1}$)	1.573	1.679
C_p ($J K^{-1}mol^{-1}$)	661.7	706.3

Name: 2,2,4,4–Tetraethyl–6,6–diphenylcyclotrisiloxane
Formula: $C_{20}H_{30}O_3Si_3$

CAS–RN: 108543–32–4
Group No.: 71–047
Molar Mass: 402.71

TABLE 71.47.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
87DZH/KUL2	281.1–315.5	10	0.50	98.1	melpt	C_p	BSAO	54STR/ICK

TABLE 71.47.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	10	10	0.061	2.30–2	0.03	8.39–6	–2
Temp. range K		A_1	A_2				Level of uncertainty
281.1–315.5		4.35929+1	1.07731+1				IV

TABLE 71.47.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300	310	320
c_p (J K^{-1}g^{-1})	1.523	1.545	1.563	1.567	1.590	1.612
C_p (J K^{-1}mol^{-1})	613.3	622.2	629.5	631.2	640.1	649.1

Name: Octamethyldiphenylcyclopentasiloxane (unspecified isomer)
Formula: $C_{20}H_{34}O_5Si_5$

CAS-RN: 51134-26-0
Group No.: 71-048
Molar Mass: 494.91

TABLE 71.48.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
77KUL/DZH1	270.0–300.0	5S	nosp	not specified		C_p	BSAO	54STR/ICK

TABLE 71.48.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.044	3.99–2	0.04	1.37–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
270.0–300.0		1.50111+2	–5.36558+1	1.14009+1			V

TABLE 71.48.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.48	1.49	1.50	1.52	1.54	1.54
C_p (J K^{-1}mol^{-1})	735	737	742	752	761	763

Name: (2α,4α,6α)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
Formula: $C_{21}H_{24}O_3Si_3$

CAS-RN: 3424-57-5
Group No.: 71-049
Molar Mass: 408.68

TABLE 71.49.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75MEK/KAR4	373.2–390.0	2S	1.00	98.54	melpt	C_p	BSAO	54STR/ICK

TABLE 71.49.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
373.2–390.0		–3.77052	2.36632+1				V

TABLE 71.49.4. Recommended values of heat capacities

Temp. (K)	380	390
c_p (J K^{-1}g^{-1})	1.75	1.80
C_p (J K^{-1}mol^{-1})	716	736

Name: (2α,4α,6β)–2,4,6–Trimethyl–2,4,6–triphenylcyclotrisiloxane
Formula: $C_{21}H_{24}O_3Si_3$

CAS–RN: 6138–53–0
Group No.: 71–050
Molar Mass: 408.68

TABLE 71.50.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
75MEK/KAR4	321.2–330.0	2S	1.00	98.26	melpt	C_p	BSAO	54STR/ICK

TABLE 71.50.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
321.2–330.0		–2.15705+2	8.97786+1				V

TABLE 71.50.4. Recommended values of heat capacities

Temp. (K)	325	330
c_p (J K^{-1}g^{-1})	1.55	1.64
C_p (J K^{-1}mol^{-1})	633	670

Name: Tetrakis(2–ethylbutyl) ester silicic acid
Formula: $C_{24}H_{52}O_4Si$

CAS–RN: 78–13–7
Group No.: 71–051
Molar Mass: 432.76

TABLE 71.51.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
74TOM/ADA	298.1	1	3.00	99.3	anal	C_p	BSIO	69STO/MAR
85NKI/CHA	298.0	1	0.30	not specified		C_p	FSIT	71PIC/LED

TABLE 71.51.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
74TOM/ADA	298.1	1	3.00	0.135	4.12–1	0.40	4.12–1	1
85NKI/CHA	298.0	1	0.30	0.013	4.09–3	0.00	–4.09–3	0

TABLE 71.51.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.135	4.12–1	0.40	2.04–1	1
Temp. range K		A_1					Level of uncertainty
298.0–298.1		1.01499+2					V

TABLE 71.51.4. Recommended values of heat capacities

Temp. (K)	298.15
c_p (J K^{-1}g^{-1})	1.95
C_p (J K^{-1}mol^{-1})	844

Name: 1,3–Dimethyl–1,1,3,3–tetraphenyldisiloxane
Formula: $C_{26}H_{26}OSi_2$

CAS–RN: 807–28–3
Group No.: 71–052
Molar Mass: 410.66

TABLE 71.52.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84KUL/DZH	321.9–340.0	3S	0.20	99.7	melpt	C_p	BSAO	54STR/ICK

TABLE 71.52.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.142	2.25–2	0.03	7.63–6	–1
Temp. range K		A_1	A_2				Level of uncertainty
321.9–340.0		4.56292+1	1.01306+1				IV

TABLE 71.52.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p (J K^{-1}g^{-1})	1.601	1.621
C_p (J K^{-1}mol^{-1})	657.3	665.8

Name: 2,2–Dimethyl–4,4,6,6–tetraphenylcyclotrisiloxane
Formula: $C_{26}H_{36}O_3Si_3$

CAS–RN: 1438–86–4
Group No.: 71–053
Molar Mass: 480.83

TABLE 71.53.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
82KUL/DZH	N	361.9–369.0	3	0.20	99.43	melpt	C_p	BSAO	54STR/ICK

82KUL/DZH only a graph given in the paper; experimental values provided by the authors

TABLE 71.53.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.791	1.53–1	0.16	1.58–4	–1

Temp. range K	A_1	A_2	Level of uncertainty
361.9–369.0	6.82540+1	7.70660	IV

TABLE 71.53.4. Recommended values of heat capacities

Temp. (K)	362	366	370
c_p (J K^{-1}g^{-1})	1.663	1.668	1.673
C_p (J K^{-1}mol^{-1})	799.5	802.0	804.6

Name: 2,2,4,4–Tetramethyl–6,6,8,8–tetraphenylcyclotetrasiloxane
Formula: $C_{28}H_{32}O_4Si_4$

CAS–RN: 1693–47–6
Group No.: 71–054
Molar Mass: 544.90

TABLE 71.54.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76KUL/DZH	345.9–370.0	4S	0.30	99.1	melpt	C_p	BSAO	54STR/ICK

TABLE 71.54.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.132	4.64–2	0.04	3.82–6	0

Temp. range K	A_1	A_2	Level of uncertainty
345.9–370.0	8.72329	3.04414+1	V

TABLE 71.54.4. Recommended values of heat capacities

Temp. (K)	350	360	370
c_p (J K^{-1}g^{-1})	1.76	1.81	1.85
C_p (J K^{-1}mol^{-1})	958	984	1010

Name: 2,4,6,8–Tetramethyl–2,4,6,8–tetraphenylcyclotetrasiloxane
Formula: $C_{28}H_{32}O_4Si_4$

CAS–RN: 77–63–4
Group No.: 71–055
Molar Mass: 544.90

TABLE 71.55.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75MEK/KAR3	373.4–390.0	2S	0.30	99.11	melpt	C_p	BSAO	54STR/ICK

TABLE 71.55.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
373.4–390.0		–4.17041+1	3.78929+1				V

TABLE 71.55.4. Recommended values of heat capacities

Temp. (K)	380	390
c_p (J $K^{-1}g^{-1}$)	1.56	1.62
C_p (J $K^{-1}mol^{-1}$)	850	882

Name: Tribenzylhexadecylsilane
Formula: $C_{37}H_{54}Si$

CAS–RN: 4033–52–7
Group No.: 71–056
Molar Mass: 526.92

TABLE 71.56.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
60BAR/BOL	313.1–513.1	5	5.00	not specified		C_p	BSIO	60BAR/BOL

TABLE 71.56.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	5	5	0.259	1.70	1.29	4.16–2	1
Temp. range K		A_1	A_2				Level of uncertainty
313.1–513.2		2.92085+1	2.50356+1				VI

TABLE 71.56.4. Recommended values of heat capacities

Temp. (K)	310	320	330	340	350	360	370
c_p ($J\,K^{-1}g^{-1}$)	1.69	1.73	1.76	1.80	1.84	1.88	1.92
C_p ($J\,K^{-1}mol^{-1}$)	888	909	930	951	971	992	1010
Temp. (K)	380	390	400	410	420	430	440
c_p ($J\,K^{-1}g^{-1}$)	1.96	2.00	2.04	2.08	2.12	2.16	2.20
C_p ($J\,K^{-1}mol^{-1}$)	1030	1050	1080	1100	1120	1140	1160
Temp. (K)	450	460	470	480	490	500	510
c_p ($J\,K^{-1}g^{-1}$)	2.24	2.28	2.32	2.36	2.40	2.44	2.48
C_p ($J\,K^{-1}mol^{-1}$)	1180	1200	1220	1240	1260	1280	1300

72. Organic Compounds Containing Phosphorus or Boron

This family contains 15 compounds, all of which were measured over a range of temperatures.

All of the measurements in this family seem to be of reasonable accuracy with the exception of hexamethylphosphoramide where the data are of lower reliability. Experimental data with the reported uncertainty 0.1 to 0.2 % were available over a wide temperature interval for 6 very pure compounds from NBSW (54FUR/PAR, 55FUR, 55FUR/MCC, 64FUR/REI). For triethylborane, the NBSW data have been supplemented with values generated from a correlating equation published in the reference (77KOS/SAM) in order to extend the upper temperature limit for the recommended values.

Another source of high quality data consists of measurements performed at BMB (70FIN/TOD) for trimethylamine borane and triethylamine borane over a narrow temperature interval and yielded data with a claimed error of 0.1 to 0.2 %.

The medium level of uncertainty has been assigned to the following sources: data for three organic phosphates from CIUG (86FAM/MAS, 86OVC/POD, 86RAB/PET), measurements on 98 % purity samples for two substances (triphenylphosphine oxide and 1,4-butanediylbis (diphenylphosphine)) from SUU (89HUI/VAN), and results for triethanolamine borate from UMAA (64CLE/WON).

For two compounds, trimethylborane and triethylborane, with a sufficiently large temperature interval of measurements, the critical temperatures were estimated as $T_c = 1.5\ T_{nb}$ because no information in literature was available and the correlation using a quasi-polynomial equation was carried out.

Name: Methylphosphonic chloride fluoride
Formula: CH_3ClFOP

CAS-RN: 753-71-9
Group No.: 72-001
Molar Mass: 116.46

TABLE 72.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64FUR/REI	257.0–332.4	7	0.10	99.65	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 72.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_{sat}	7	7	0.369	6.75–3	0.04	1.91–6	–2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
257.0–332.4		1.69488+1	7.57670–2	1.40184–1			II

TABLE 72.1.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_{sat} (J K^{-1}g^{-1})	1.292	1.298	1.299	1.304	1.310	1.315	1.316
C_{sat} (J K^{-1}mol^{-1})	150.4	151.1	151.3	151.8	152.6	153.2	153.3
Temp. (K)	310	320	330				
c_{sat} (J K^{-1}g^{-1})	1.323	1.330	1.337				
C_{sat} (J K^{-1}mol^{-1})	154.1	154.9	155.7				

Name: Methylphosphonic dichloride
Formula: CH_3Cl_2OP

CAS–RN: 676–97–1
Group No.: 72–002
Molar Mass: 132.91

TABLE 72.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64FUR/REI	311.8–329.7	7	0.10	99.992	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 72.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	7	7	1.339	2.63–2	0.13	5.01–5	–3
Temp. range K		A_1	A_2				Level of uncertainty
311.8–329.6		1.79636+1	5.07772–1				II

TABLE 72.2.4. Recommended values of heat capacities

Temp. (K)	310	320	330
c_{sat} (J $K^{-1}g^{-1}$)	1.222	1.225	1.229
C_{sat} (J $K^{-1}mol^{-1}$)	162.4	162.9	163.3

Name: Methylphosphonic difluoride
Formula: CH_3F_2OP

CAS–RN: 676–99–3
Group No.: 72–003
Molar Mass: 100.00

TABLE 72.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64FUR/REI	238.4–333.9	19	0.10	99.89	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 72.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	19	19	0.234	3.99–3	0.02	2.51–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
238.4–333.9		1.98306+1	–4.11377	1.55964	–1.49755–1		II

TABLE 72.3.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_{sat} (J K^{-1}g^{-1})	1.403	1.410	1.417	1.426	1.428	1.434	1.444
C_{sat} (J K^{-1}mol^{-1})	140.3	141.0	141.7	142.6	142.8	143.4	144.4
Temp. (K)	298.15	300	310	320	330		
c_{sat} (J K^{-1}g^{-1})	1.452	1.454	1.464	1.474	1.485		
C_{sat} (J K^{-1}mol^{-1})	145.2	145.4	146.4	147.4	148.5		

Name: (Dimethylamino)diborane(6)
Formula: $C_2H_{11}B_2N$

CAS–RN: 22580–01–4
Group No.: 72–004
Molar Mass: 70.74

TABLE 72.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55FUR/MCC	221.0–284.9	20	0.20	99.94	melpt	C_{sat}	BSAO	45SCO/MEY

TABLE 72.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	20	20	0.327	1.17–2	0.07	1.33–5	1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
221.0–284.9		1.57126+1	–1.54443	9.86748–1			II

TABLE 72.4.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_{sat} (J K^{-1}g^{-1})	2.009	2.043	2.079	2.118	2.159	2.202	2.216
C_{sat} (J K^{-1}mol^{-1})	142.1	144.5	147.1	149.8	152.7	155.8	156.8
Temp. (K)	280						
c_{sat} (J K^{-1}g^{-1})	2.248						
C_{sat} (J K^{-1}mol^{-1})	159.0						

Name: Trimethylborane
Formula: C_3H_9B

CAS–RN: 593–90–8
Group No.: 72–005
Molar Mass: 55.92

TABLE 72.5.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54FUR/PAR	N	116.2–215.3	30	0.20	99.9	melpt	C_{sat}	BSAO	33SOU/BRI

54FUR/PAR three data points measured with another sample (impurity 0.3 mol.%)

TABLE 72.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	0.571	1.58–2	0.11	3.16–5	–7
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
116.2–215.4		1.64373+1	–6.83592	4.01462	–6.19155–1		II

TABLE 72.5.4. Recommended values of heat capacities

Temp. (K)	120	130	140	150	160	170	180
c_{sat} (J K^{-1}g^{-1})	1.925	1.929	1.939	1.952	1.969	1.989	2.012
C_{sat} (J K^{-1}mol^{-1})	107.6	107.9	108.4	109.1	110.1	111.2	112.5
Temp. (K)	190	200	210	220			
c_{sat} (J K^{-1}g^{-1})	2.036	2.063	2.090	2.117			
C_{sat} (J K^{-1}mol^{-1})	113.9	115.3	116.8	118.4			

TABLE 72.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	30	30	1.048	2.79–2	0.21	1.03–4	–2
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
116.2–215.4	378.80	5.06079	3.72504	8.85334	1.71888		II

Name: Trimethylamineborane
Formula: $C_3H_{12}BN$

CAS–RN: 75–22–9
Group No.: 72–006
Molar Mass: 72.95

TABLE 72.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
70FIN/TOD	373.0–380.1	4	0.10	99.94	melpt	C_{sat}	BSAO	47HUF

TABLE 72.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	0.431	2.10–2	0.09	1.91–5	0
Temp. range K		A_1	A_2				Level of uncertainty
373.0–380.1		1.40393+1	2.74046				II

TABLE 72.6.4. Recommended values of heat capacities

Temp. (K)	370	380
c_{sat} (J K^{-1}g^{-1})	2.756	2.787
C_{sat} (J K^{-1}mol^{-1})	201.0	203.3

Name: 2,8,9–Trioxa–5–aza–1–borabicyclo[3.3.3]undecane
Formula: $C_6H_{12}BNO_3$

CAS–RN: 283–56–7
Group No.: 72–007
Molar Mass: 156.98

TABLE 72.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
64CLE/WON	516.3–523.1	4	0.25	99.6	melpt	C_{sat}	BSAO	68WES/WES

TABLE 72.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	4	4	1.270	1.41–1	0.32	4.46–4	–1
Temp. range K		A_1	A_2				Level of uncertainty
516.3–523.1		1.34918+1	5.91091				III

TABLE 72.7.4. Recommended values of heat capacities

Temp. (K)	515	520	525
c_{sat} (J K^{-1}g^{-1})	2.327	2.343	2.358
C_{sat} (J K^{-1}mol^{-1})	365.3	367.7	370.2

Name: 2–Chloroethanol phosphate (3:1)
Formula: $C_6H_{12}Cl_3O_4P$

CAS–RN: 115–96–8
Group No.: 72–008
Molar Mass: 285.49

TABLE 72.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86FAM/MAS	190.0–300.0	8S	0.30	not specified		C_p	BSAO	76LEB/LIT

TABLE 72.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	8	8	0.279	3.82–2	0.08	3.77–5	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
190.0–300.0		4.59020+1	–2.28282	9.67028–1			III

TABLE 72.8.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.312	1.317	1.321	1.327	1.333	1.339	1.347
C_p (J K^{-1}mol^{-1})	374.6	375.9	377.3	378.8	380.5	382.4	384.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.354	1.363	1.365	1.371	1.381	1.389	1.391
C_p (J K^{-1}mol^{-1})	386.7	389.0	389.8	391.5	394.2	396.5	397.1

Name: Triethylborane
Formula: $C_6H_{15}B$

CAS-RN: 97-94-9
Group No.: 72-009
Molar Mass: 98.00

TABLE 72.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
55FUR	184.5–290.6	29	nosp	98.	melpt	C_{sat}	BSAO	45SCO/MEY
77KOS/SAM	180.0–322.0	eqn	nosp	not specified		C_{sat}	BSAO	54STR/ICK

TABLE 72.9.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
55FUR	184.5–290.6	29	0.20#	0.889	5.02–2	0.18	1.42–2	6
77KOS/SAM	180.0–322.5	20	0.50#	1.010	1.42–1	0.51	–1.26–1	–18

TABLE 72.9.3. Parameters of regression polynomial

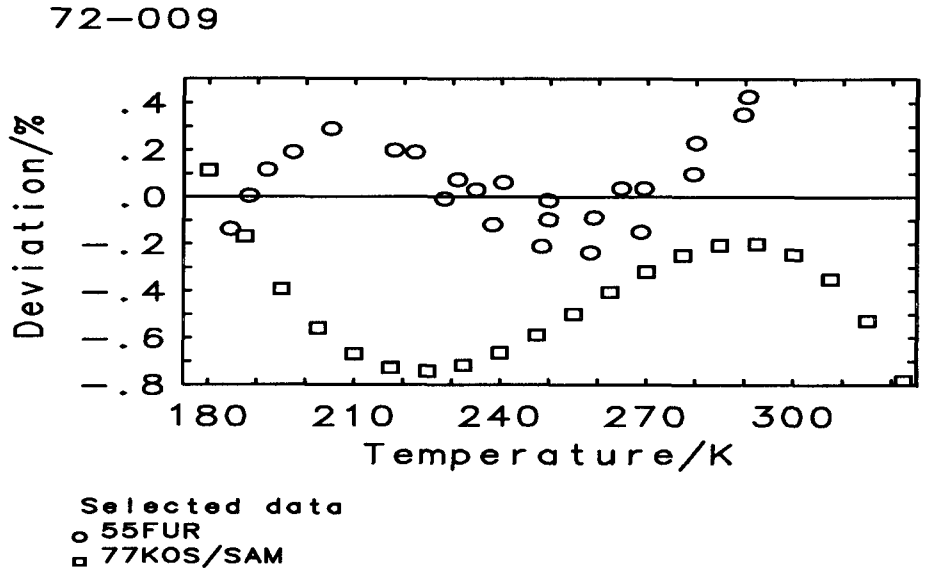
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	49	49	0.981	1.03–1	0.37	–4.29–2	–12
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
180.0–322.5		–5.14480	3.50181+1	–1.24037+1	1.50544		III

TABLE 72.9.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_{sat} (J K^{-1}g^{-1})	2.247	2.286	2.318	2.345	2.366	2.384	2.398
C_{sat} (J K^{-1}mol^{-1})	220.2	224.0	227.2	229.8	231.9	233.6	235.0
Temp. (K)	250	260	270	273.15	280	290	298.15
c_{sat} (J K^{-1}g^{-1})	2.410	2.419	2.428	2.430	2.436	2.444	2.452
C_{sat} (J K^{-1}mol^{-1})	236.1	237.1	237.9	238.2	238.7	239.5	240.3
Temp. (K)	300	310	320				
c_{sat} (J K^{-1}g^{-1})	2.454	2.466	2.480				
C_{sat} (J K^{-1}mol^{-1})	240.5	241.6	243.0				

TABLE 72.9.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	49	49	1.376	1.06–1	0.38	3.58–3	–3
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
180.0–322.5	552.00	1.17126+2	2.42894+1	–9.30575	1.41197+2		IV



Name: Triethylamineborane
Formula: $C_6H_{18}BN$

CAS–RN: 1722–26–5
Group No.: 72–010
Molar Mass: 115.03

TABLE 72.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
67SMI/GOO1	298.1	1	nosp	99.995	melpt	C_p	not specified	
70FIN/TOD	268.5–305.3	6	0.10	99.995	melpt	C_{sat}	BSAO	47HUF

TABLE 72.10.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
67SMI/GOO1	298.1	1	0.20#	0.157	9.68–3	0.03	–9.68–3	–1
70FIN/TOD	268.5–305.3	6	0.20#	0.059	3.59–3	0.01	1.62–3	0

TABLE 72.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C	7	7	0.106	6.54–3	0.02	1.91–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
268.5–305.3		1.87060+1	2.37813	5.76309–1			II

TABLE 72.10.4. Recommended values of heat capacities

Temp. (K)	270	273.15	280	290	298.15	300	310
c ($J K^{-1} g^{-1}$)	2.120	2.132	2.160	2.201	2.235	2.243	2.285
C ($J K^{-1} mol^{-1}$)	243.8	245.3	248.5	253.2	257.1	258.0	262.9

Name: Hexamethyl phosphoric triamide
Formula: $C_6H_{18}N_3OP$

CAS–RN: 680–31–9
Group No.: 72–011
Molar Mass: 179.20

TABLE 72.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
73MOS/NIK	280.0–298.1	2S	nosp	97.7	melpt	C_p	BSAO	66NIK/LEB
82VOR/YAK	298.1	1	nosp	not specified		C_p	BSAO	77VOR/PRI

TABLE 72.11.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
73MOS/NIK	280.0–298.1	2	0.70#	0.000	0.00	0.00	0.00	0
				Rejected data				
82VOR/YAK	(1.81, 4.70,–1.81, –1)							

TABLE 72.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
280.0–298.1		2.55792+1	4.99059				V

TABLE 72.11.4. Recommended values of heat capacities

Temp. (K)	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.84	1.86	1.88	1.88
C_p ($J K^{-1} mol^{-1}$)	329	333	336	337

Name: Triphenylphosphine oxide
Formula: $C_{18}H_{15}OP$

CAS-RN: 791-28-6
Group No.: 72-012
Molar Mass: 278.29

TABLE 72.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89HUI/VAN	434.0–459.0	4	nosp	98.	anal	C_p	BDCT	86MER/BEN

TABLE 72.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.015	2.71–2	0.04	1.05–5	0
Temp. range K		A_1	A_2				Level of uncertainty
434.0–459.0		3.50752+1	5.83204				V

TABLE 72.12.4. Recommended values of heat capacities

Temp. (K)	430	440	450	460
c_p ($J K^{-1}g^{-1}$)	1.80	1.81	1.83	1.85
C_p ($J K^{-1}mol^{-1}$)	500	505	510	515

Name: Triphenyl ester phosphoric acid
Formula: $C_{18}H_{15}O_4P$

CAS-RN: 115-86-6
Group No.: 72-013
Molar Mass: 326.29

TABLE 72.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86RAB/PET	322.5–340.6	7	0.30	99.7	melpt	C_p	BSAO	76LEB/LIT

TABLE 72.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.222	3.81–2	0.07	3.60–5	1
Temp. range K		A_1	A_2				Level of uncertainty
322.5–340.6		5.20781+1	1.55506				III

TABLE 72.13.4. Recommended values of heat capacities

Temp. (K)	330	340
c_p ($J K^{-1}g^{-1}$)	1.458	1.462
C_p ($J K^{-1}mol^{-1}$)	475.7	477.0

Name: Tris(methylphenyl)ester phosphoric acid
Formula: $C_{21}H_{21}O_4P$

CAS-RN: 1330-78-5
Group No.: 72-014
Molar Mass: 368.37

TABLE 72.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
86OVC/POD	211.0–320.1	30	0.20	not specified		C_p	BSAO	76LEB/LIT

TABLE 72.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	30	30	0.763	9.84-2	0.15	2.60-4	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
211.0–320.1		4.89782+1	1.29929	1.87270			III

TABLE 72.14.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1}g^{-1}$)	1.353	1.375	1.397	1.419	1.443	1.467	1.493
C_p ($J K^{-1}mol^{-1}$)	498.6	506.4	514.4	522.8	531.6	540.6	549.9
Temp. (K)	273.15	280	290	298.15	300	310	320
c_p ($J K^{-1}g^{-1}$)	1.501	1.519	1.546	1.569	1.574	1.603	1.632
C_p ($J K^{-1}mol^{-1}$)	552.9	559.6	569.5	577.9	579.8	590.4	601.2

Name: 1,4-Butanediylbis(diphenylphosphine)
Formula: $C_{28}H_{28}P$

CAS-RN: 7688-25-7
Group No.: 72-015
Molar Mass: 395.50

TABLE 72.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89HUI/VAN	414.0–444.0	7	nosp	98.	anal	C_p	BDCT	86MER/BEN

TABLE 72.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	7	7	0.012	2.27-2	0.04	1.03-5	-1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
414.0–444.0		-9.90720+1	6.73577+1	-6.86931			V

TABLE 72.15.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440
c_p ($J K^{-1}g^{-1}$)	1.30	1.32	1.34	1.35
C_p ($J K^{-1}mol^{-1}$)	512	521	528	535

73. Organometallic Compounds

This family contains 32 compounds, all of which were measured over a range of temperatures.

The main part of the data, amounting to 25 compounds, was obtained at CIUG. Data for three compounds (diethylzinc, teramethylstannane and tetraethylgermane) measured at CIUG are also available from other laboratories. Diethylzinc was measured at CIUG (88RAB/NIS) with a reported uncertainty of 0.2 % over a wide temperature range and at ICG (87GIB/GRI) with the same claimed error but using a sample of higher purity. Data from CIUG are by 3-4 % higher over the whole temperature interval. We have included both sets of data in the correlation as it was not possible to decide unequivocally which data set was more reliable. Data for tetramethylstannane measured at CIUG (72MAS/RAB) have a reported uncertainty of 0.4 %. Measurements on tetramethylstannane carried out at ICLO (54STA/WAR) gave data with a reported uncertainty of 1 %. The results of the combined correlation of both data sets showed good agreement for these two sources. Tetraethylgermane was measured at CIUG twice and the earlier data (72MAS/RAB) are by 2 to 5 % higher than the more recent measurements by (85RAB/SHE) in which a sample of higher purity was used. The experimental data of (54STA/WAR) for this compound have been rejected from the correlation due to large deviations from the two CIUG data sets.

A very distinct minimum on the heat capacity curve $C=f(T)$ (located several tens of kelvin above the melting temperature) was observed for some alkylselenides, alkyltellurides and complexes containing alkylselenides and alkyltellurides. Altogether six compounds of this kind were measured at CIUG (90LEB/KUL, 91RAB/SHE, 92LEB/KUL2).

Apart from the CIUG data there are only three more reliable measurements: dimethylcadmium from UCB (56LI) measured over a narrow temperature interval (13 K), and results over a wider temperature range for tetramethylgermane by RUH (70VAL/KIL) and for trimethylaluminium from studies by BMB (63MCC/MES). For trimethylaluminium and tetraethyllead (measured at CIUG, 89RAB/NIS1), we have estimated the critical temperature from the value of the normal boiling temperature and calculated parameters of the quasi-polynomial extrapolation equation.

Name: Dimethylcadmium
Formula: C_2H_6Cd

CAS-RN: 506-82-1
Group No.: 73-001
Molar Mass: 142.48

TABLE 73.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
56LI	278.9–291.3	5	0.20	99.99	melpt	C_p	BSIO	37GIA/EGA

TABLE 73.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	5	5	0.440	1.39–2	0.09	1.51–5	1
Temp. range K		A_1	A_2				Level of uncertainty
278.9–291.3		1.37638+1	7.11839–1				II

TABLE 73.1.4. Recommended values of heat capacities

Temp. (K)	280	290
c_p ($J K^{-1} g^{-1}$)	0.920	0.924
C_p ($J K^{-1} mol^{-1}$)	131.0	131.6

Name: Selenobismethane
Formula: C_2H_6Se

CAS–RN: 593–79–3
Group No.: 73–002
Molar Mass: 109.03

TABLE 73.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91RAB/SHE	189.4–298.8	24	0.20	99.98	melpt	C_p	BSAO	66NIK/LEB

TABLE 73.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	24	0.815	2.34–2	0.16	6.73–5	–3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
189.4–298.8		2.06311+1	–5.66694	1.22133			II

TABLE 73.2.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J\,K^{-1}g^{-1}$)	1.088	1.082	1.077	1.073	1.072	1.073	1.075
C_p ($J\,K^{-1}mol^{-1}$)	118.7	117.9	117.4	117.0	116.9	116.9	117.2
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J\,K^{-1}g^{-1}$)	1.079	1.085	1.088	1.093	1.103	1.113	1.115
C_p ($J\,K^{-1}mol^{-1}$)	117.7	118.3	118.6	119.2	120.3	121.3	121.6

Name: Dimethyl diselenide
Formula: $C_2H_6Se_2$

CAS–RN: 7101–31–7
Group No.: 73–003
Molar Mass: 187.99

TABLE 73.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
91RAB/SHE	192.1–300.4	46	0.20	99.86	melpt	C_p	BSAO	66NIK/LEB

TABLE 73.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	46	46	0.879	3.34–2	0.18	1.11–4	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
192.1–300.4		4.47122+1	–2.75923+1	9.76155	–1.15357		II

TABLE 73.3.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	0.856	0.846	0.839	0.834	0.830	0.828	0.826
C_p (J K^{-1}mol^{-1})	160.8	159.1	157.7	156.8	156.1	155.6	155.4
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	0.826	0.826	0.825	0.825	0.825	0.825	
C_p (J K^{-1}mol^{-1})	155.2	155.2	155.2	155.1	155.0	155.0	

Name: Dimethylzinc
Formula: C_2H_6Zn

CAS-RN: 544-97-8
Group No.: 73-004
Molar Mass: 95.46

TABLE 73.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84SHE/NIS	250.0–298.1	2S	0.20	99.983	melpt	C_p	BSAO	80GUR/GAV

TABLE 73.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1	A_2				Level of uncertainty
250.0–298.1		1.07728+1	1.59862				III

TABLE 73.4.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.286	1.300	1.314	1.319	1.328	1.342	1.353
C_p (J K^{-1}mol^{-1})	122.8	124.1	125.5	125.9	126.8	128.1	129.2
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	1.356						
C_p (J K^{-1}mol^{-1})	129.4						

Name: Trimethylaluminium
Formula: C_3H_9Al

CAS-RN: 75-24-1
Group No.: 73-005
Molar Mass: 72.09

TABLE 73.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
63MCC/MES	295.1–377.6	10	0.20	99.81	melpt	C_{sat}	BSAO	47HUF

TABLE 73.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.116	4.54–3	0.02	1.53–6	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
295.1–377.6		1.42590+1	2.33255–1	4.23041–1			II

TABLE 73.5.4. Recommended values of heat capacities

Temp. (K)	290	298.15	300	310	320	330	340
c_{sat} (J K^{-1}g^{-1})	2.133	2.159	2.165	2.197	2.230	2.265	2.300
C_{sat} (J K^{-1}mol^{-1})	153.8	155.6	156.0	158.4	160.8	163.3	165.8
Temp. (K)	350	360	370	380			
c_{sat} (J K^{-1}g^{-1})	2.337	2.374	2.412	2.451			
C_{sat} (J K^{-1}mol^{-1})	168.4	171.1	173.9	176.7			

TABLE 73.5.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_{sat}	10	10	0.141	5.46–3	0.03	2.29–6	1
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
295.1–377.6	600.40	–3.71800	4.55878–1	1.14920+1	7.58071		II

Name: Trimethylarsine
Formula: C_3H_9As

CAS-RN: 593–88–4
Group No.: 73–006
Molar Mass: 120.03

TABLE 73.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
88NIS/SHE	191.8–309.8	38	0.20	99.972	melpt	C_p	BSAO	85RAB/SHE

TABLE 73.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	38	38	1.639	5.90–2	0.33	3.56–4	–1
Temp. range K		A_1	A_2	A_3			Level of uncertainty
191.8–309.8		1.23652+1	2.99887	–3.17527–1			III

TABLE 73.6.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p ($J K^{-1}g^{-1}$)	1.172	1.184	1.196	1.207	1.218	1.228	1.238
C_p ($J K^{-1}mol^{-1}$)	140.7	142.1	143.5	144.9	146.2	147.4	148.6
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1}g^{-1}$)	1.248	1.257	1.260	1.266	1.274	1.280	1.282
C_p ($J K^{-1}mol^{-1}$)	149.8	150.9	151.2	151.9	152.9	153.7	153.9
Temp. (K)	310						
c_p ($J K^{-1}g^{-1}$)	1.289						
C_p ($J K^{-1}mol^{-1}$)	154.7						

Name: Trimethylgallium
Formula: C_3H_9Ga

CAS-RN: 1445-79-0
Group No.: 73-007
Molar Mass: 114.83

TABLE 73.7.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73MAS/NOV	260.0–298.1	5S	0.50	99.75	melpt	C_p	BSAO	66NIK/LEB
88LEB/SMI	257.8–330.0	10S	0.20	99.923	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.7.2. Correlated heat capacities

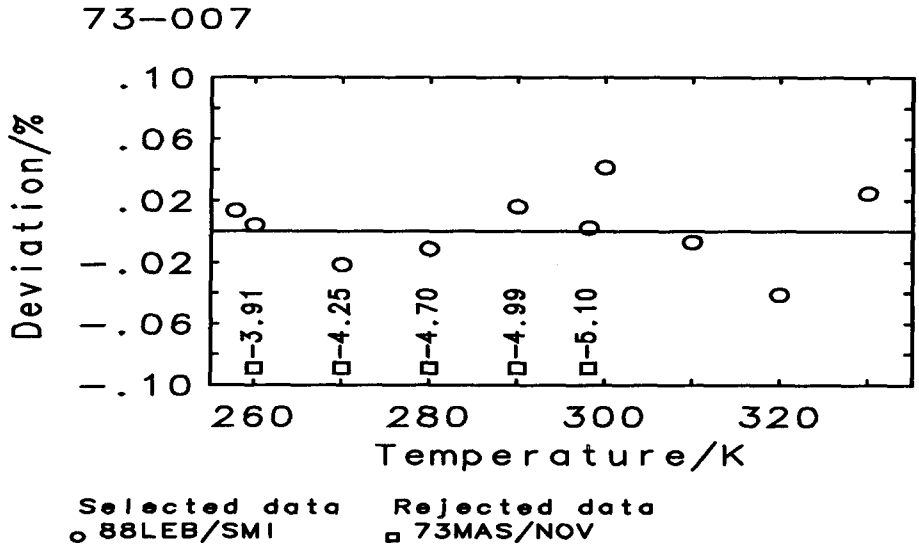
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
88LEB/SMI	257.8–330.0	10	0.20	0.112	5.12–3	0.02	1.72–6	1
				Rejected data				
73MAS/NOV	(9.95–1, 4.61,–9.90–1, –5)							

TABLE 73.7.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	10	0.145	6.61–3	0.03	1.72–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
257.8–330.0		1.92465+1	7.76908	–4.33975	7.08526–1		II

TABLE 73.7.4. Recommended values of heat capacities

Temp. (K)	260	270	273.15	280	290	298.15	300
c_p ($J K^{-1} g^{-1}$)	1.634	1.632	1.631	1.631	1.634	1.637	1.638
C_p ($J K^{-1} mol^{-1}$)	187.6	187.3	187.3	187.3	187.6	188.0	188.1
Temp. (K)	310	320	330				
c_p ($J K^{-1} g^{-1}$)	1.646	1.657	1.672				
C_p ($J K^{-1} mol^{-1}$)	189.0	190.3	192.0				



Name: Diethylmercury
Formula: $C_4H_{10}Hg$

CAS–RN: 627–44–1
Group No.: 73–008
Molar Mass: 258.71

TABLE 73.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78BUR/KAM	181.4–298.1	4S	0.20	99.73	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.906	3.55–2	0.18	2.67–5	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
181.4–298.1		1.83751+1	–9.25015–1	7.10286–1			III

TABLE 73.8.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	.616	0.622	0.629	0.636	0.643	0.651	0.659
C_p (J K^{-1}mol^{-1})	159.5	161.0	162.7	164.4	166.3	168.3	170.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	0.668	0.677	0.680	0.686	0.696	0.705	0.707
C_p (J K^{-1}mol^{-1})	172.7	175.1	175.8	177.5	180.1	182.3	182.9

Name: 2,2'-Selenodiethanol
Formula: $C_4H_{10}O_2Se$

CAS-RN: 27974-49-8
Group No.: 73-009
Molar Mass: 169.08

TABLE 73.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
83GEI/GUS	224.4-300.5	28	0.30	not specified		C_p	BSAO	54STR/ICK

TABLE 73.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	28	28	0.475	1.27-1	0.33	8.43-4	7
Temp. range K		A_1	A_2				Level of uncertainty
224.4-300.5		1.99722+1	7.39413				IV

TABLE 73.9.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.818	1.855	1.891	1.927	1.964	1.975	2.000
C_p (J K^{-1}mol^{-1})	307.5	313.6	319.8	325.9	332.1	334.0	338.2
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	2.037	2.066	2.073				
C_p (J K^{-1}mol^{-1})	344.3	349.4	350.5				

Name: Diethylzinc
Formula: $C_4H_{10}Zn$

CAS-RN: 557-20-0
Group No.: 73-010
Molar Mass: 123.51

TABLE 73.10.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
87GIB/GRI	248.8-269.7	9	0.20	99.86	melpt	C_p	BSAO	86DEV/GUS
88RAB/NIS	245.6-300.4	20	0.20	99.07	melpt	C_p	BSAO	85RAB/SHE

TABLE 73.10.2. Correlated heat capacities

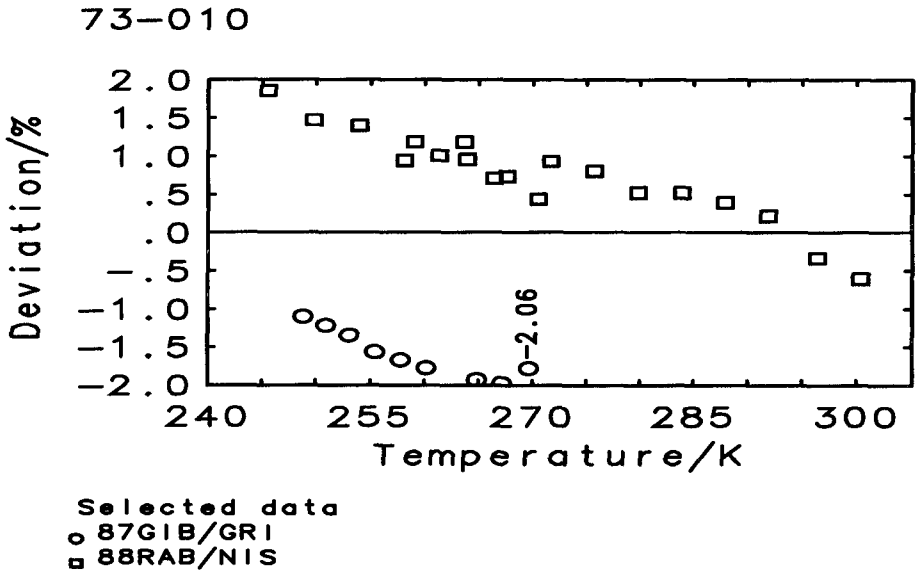
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
87GIB/GRI	248.8–269.7	9	0.20	8.310	3.60–1	1.66	–3.53–1	–9
88RAB/NIS	245.6–300.4	20	0.20	4.708	2.10–1	0.94	1.68–1	16

TABLE 73.10.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	29	29	6.400	2.81–1	1.28	6.46–3	7
Temp. range K		A_1	A_2	A_3			Level of uncertainty
245.6–300.4		1.51092+1	1.73787	3.53236–1			V

TABLE 73.10.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.43	1.46	1.48	1.51	1.51	1.53	1.56
C_p (J K^{-1}mol^{-1})	177	180	183	186	187	189	192
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.58	1.58					
C_p (J K^{-1}mol^{-1})	195	195					



Name: Dimethyl[selenobis(methane)]cadmium
Formula: $C_4H_{12}CdSe$

CAS–RN: 143481–65–6
Group No.: 73–011
Molar Mass: 251.51

TABLE 73.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
92LEB/KUL2	211.7–310.4	26	0.20	99.77	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	26	24	1.064	6.95–2	0.21	2.47–4	–6

Temp. range K	A_1	A_2	A_3	A_4	Level of uncertainty
211.7–310.4	–6.15678	4.76636+1	–1.97721+1	2.76065	III

TABLE 73.11.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1} g^{-1}$)	1.068	1.071	1.073	1.075	1.076	1.079	1.082
C_p ($J K^{-1} mol^{-1}$)	268.6	269.4	269.9	270.3	270.7	271.3	272.2
Temp. (K)	273.15	280	290	298.15	300	310	
c_p ($J K^{-1} g^{-1}$)	1.084	1.087	1.095	1.103	1.105	1.118	
C_p ($J K^{-1} mol^{-1}$)	272.5	273.5	275.3	277.4	277.9	281.3	

Name: Dimethyl[tellurobis(methane)]cadmium
Formula: $C_4H_{12}CdTe$

CAS–RN: 143481–66–7
Group No.: 73–012
Molar Mass: 300.15

TABLE 73.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
92LEB/KUL2	213.0–299.8	35	0.20	99.88	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	35	34	0.673	4.43–2	0.13	1.08–4	3

Temp. range K	A_1	A_2	A_3	Level of uncertainty
213.0–299.8	3.68982+1	–3.45200	7.30537–1	III

TABLE 73.12.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	0.910	0.909	0.909	0.910	0.910	0.911	0.912
C_p (J K^{-1}mol^{-1})	273.0	272.9	272.9	273.0	273.2	273.6	273.7
Temp. (K)	280	290	298.15	300			
c_p (J K^{-1}g^{-1})	0.913	0.915	0.917	0.917			
C_p (J K^{-1}mol^{-1})	274.0	274.6	275.2	275.4			

Name: Tetramethylgermane
Formula: $C_4H_{12}Ge$

CAS–RN: 865–52–1
Group No.: 73–013
Molar Mass: 132.75

TABLE 73.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
70VAL/KIL	188.6–304.7	23	0.30	99.988	melpt	C_p	BSIO	55TAY/JOH

TABLE 73.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	23	23	0.203	1.36–2	0.06	1.38–5	3
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
188.6–304.7	2.96450+1	−1.36631+1	6.05909	−7.22209−1			II

TABLE 73.13.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.291	1.301	1.314	1.329	1.346	1.364	1.382
C_p (J K^{-1}mol^{-1})	171.3	172.8	174.5	176.5	178.6	181.0	183.5
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.402	1.422	1.429	1.443	1.463	1.480	1.484
C_p (J K^{-1}mol^{-1})	186.1	188.8	189.7	191.5	194.3	196.5	197.0

Name: Tetramethylplumbane
Formula: $C_4H_{12}Pb$

CAS–RN: 75–74–1
Group No.: 73–014
Molar Mass: 267.34

TABLE 73.14.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54STA/WAR	250.0–260.0	2S	nosp	99.76	melpt	C_p	BSAO	49STA/GUP
59GOO/SCO	298.1	1	nosp	99.6	melpt	C_p	BSAO	43RUE/HUF

TABLE 73.14.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54STA/WAR	250.0–260.0	2	0.80#	1.007	1.92–1	0.81	2.62–2	0
59GOO/SCO	298.1	1	0.20#	0.059	2.89–3	0.01	–2.89–3	–1

TABLE 73.14.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	1.426	2.71–1	1.14	1.65–2	–1
Temp. range K		A_1	A_2				Level of uncertainty
250.0–298.1		1.99328+1	1.48246				IV

TABLE 73.14.4. Recommended values of heat capacities

Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	0.735	0.740	0.744	0.746	0.749	0.754	0.757
C_p (J K^{-1}mol^{-1})	196.5	197.8	199.0	199.4	200.2	201.5	202.5
Temp. (K)	300						
c_p (J K^{-1}g^{-1})	0.758						
C_p (J K^{-1}mol^{-1})	202.7						

Name: Dimethyl[selenobis(methane)]zinc
Formula: $C_4H_{12}SeZn$

CAS-RN: 108430-95-1
Group No.: 73-015
Molar Mass: 204.49

TABLE 73.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90LEB/KUL	227.6–329.1	35	0.20	99.88	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	35	34	1.378	9.45–2	0.28	4.67–4	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
227.6–329.1		–5.69135	4.69843+1	–1.88380+1	2.54892		III

TABLE 73.15.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.372	1.374	1.377	1.379	1.383	1.384	1.388
C_p (J K^{-1}mol^{-1})	280.5	281.0	281.5	282.1	282.8	283.0	283.8
Temp. (K)	290	298.15	300	310	320	330	
c_p (J K^{-1}g^{-1})	1.395	1.402	1.404	1.417	1.435	1.456	
C_p (J K^{-1}mol^{-1})	285.2	286.8	287.2	289.9	293.3	297.8	

Name: Tetramethylstannane
Formula: $C_4H_{12}Sn$

CAS–RN: 594–27–4
Group No.: 73–016
Molar Mass: 178.85

TABLE 73.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54STA/WAR	220.0–230.0	2S	1.00	99.74	melpt	C_p	BSAO	49STA/GUP
89SHE/RAB	222.3–305.4	31	0.20	99.921	melpt	C_p	BSAO	85RAB/SHE

TABLE 73.16.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
89SHE/RAB	222.3–305.4	26	0.20	0.761	3.41–2	0.15	1.04–4	3
				Rejected data				
54STA/WAR	(3.63–1, 1.63, 3.63–1, 1)							

TABLE 73.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	33	26	0.809	3.63–2	0.16	1.04–4	3
Temp. range K		A_1	A_2	A_3			Level of uncertainty
222.3–305.4		1.98848+1	–6.53532–1	6.61260–1			II

TABLE 73.16.4. Recommended values of heat capacities

Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	1.006	1.017	1.029	1.041	1.053	1.066	1.071
C_p (J K^{-1}mol^{-1})	180.0	181.9	184.0	186.1	188.4	190.7	191.5
Temp. (K)	280	290	298.15	300	310		
c_p (J K^{-1}g^{-1})	1.080	1.095	1.107	1.110	1.126		
C_p (J K^{-1}mol^{-1})	193.2	195.8	198.0	198.5	201.3		

Name: Dimethyl[tellurobis(methane)]zinc
Formula: $C_4H_{12}TeZn$

CAS-RN: 127283-03-8
Group No.: 73-017
Molar Mass: 253.13

TABLE 73.17.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
90LEB/KUL	200.6-301.4	34	0.20	99.42	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.17.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	34	32	0.555	3.77-2	0.11	7.62-5	4
Temp. range K		A_1	A_2	A_3			Level of uncertainty
200.6-301.4		4.47557+1	-8.51998	1.66889			III

TABLE 73.17.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p ($J K^{-1} g^{-1}$)	1.130	1.124	1.120	1.116	1.114	1.113	1.113
C_p ($J K^{-1} mol^{-1}$)	285.9	284.6	283.4	282.6	282.0	281.7	281.7
Temp. (K)	270	273.15	280	290	298.15	300	
c_p ($J K^{-1} g^{-1}$)	1.114	1.115	1.116	1.120	1.123	1.124	
C_p ($J K^{-1} mol^{-1}$)	282.0	282.2	282.6	283.4	284.3	284.5	

Name: Triethylaluminium
Formula: $C_6H_{15}Al$

CAS-RN: 97-93-8
Group No.: 73-018
Molar Mass: 114.17

TABLE 73.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89RAB/NIS2	230.3-312.9	26	0.20	99.05	melpt	C_p	BSAO	85RAB/SHE

TABLE 73.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	26	26	1.308	7.41-2	0.26	3.46-4	5
Temp. range K		A_1	A_2	A_3			Level of uncertainty
230.3-312.9		2.66710+1	-2.86447	1.19682			III

TABLE 73.18.4. Recommended values of heat capacities

Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.924	1.944	1.966	1.989	2.015	2.023	2.042
C_p (J K^{-1}mol^{-1})	219.6	221.9	224.4	227.1	230.0	230.9	233.1
Temp. (K)	290	298.15	300	310			
c_p (J K^{-1}g^{-1})	2.070	2.095	2.101	2.133			
C_p (J K^{-1}mol^{-1})	236.4	239.2	239.9	243.6			

Name: Triethylarsine
Formula: $C_6H_{15}As$

CAS–RN: 617–75–4
Group No.: 73–019
Molar Mass: 162.11

TABLE 73.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72MAS/FAM	190.0–300.0	13S	0.40	98.4	melpt	C_p	BSAO	56POP/KOL

TABLE 73.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	13	13	0.162	1.73–2	0.06	1.45–5	2
Temp. range K		A_1	A_2	A_3			Level of uncertainty
190.0–300.0		2.38884+1	–7.68215–1	7.91682–1			III

able 73.19.4. Recommended values of heat capacities

Temp. (K)	190	200	210	220	230	240	250
c_p (J K^{-1}g^{-1})	1.297	1.309	1.322	1.335	1.349	1.365	1.381
C_p (J K^{-1}mol^{-1})	210.2	212.2	214.2	216.4	218.8	221.2	223.8
Temp. (K)	260	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.397	1.415	1.421	1.433	1.452	1.469	1.472
C_p (J K^{-1}mol^{-1})	226.5	229.4	230.3	232.3	235.5	238.1	238.7

Name: Triethylbismuthine
Formula: $C_6H_{15}Bi$

CAS–RN: 617–77–6
Group No.: 73–020
Molar Mass: 296.17

TABLE 73.20.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
89NIS/RAB	147.7–328.7	41	0.20	99.69	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.20.3. Parameters of cubic spline polynomials

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	41	41	1.085	6.09–2	0.22	2.34–4	–3
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
147.7–250.0		3.67825+1	–1.74493+1	8.43419	–1.16324		II
250.0–328.7		–5.58764–1	2.73602+1	–9.48960	1.22660		II

TABLE 73.20.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p (J K^{-1}g^{-1})	0.720	0.721	0.724	0.728	0.733	0.739	0.746
C_p (J K^{-1}mol^{-1})	213.3	213.6	214.3	215.5	217.0	218.8	220.8
Temp. (K)	220	230	240	250	260	270	273.15
c_p (J K^{-1}g^{-1})	0.753	0.761	0.769	0.778	0.786	0.794	0.796
C_p (J K^{-1}mol^{-1})	223.1	225.4	227.9	230.3	232.7	235.1	235.9
Temp. (K)	280	290	298.15	300	310	320	330
c_p (J K^{-1}g^{-1})	0.802	0.811	0.819	0.821	0.831	0.843	0.855
C_p (J K^{-1}mol^{-1})	237.6	240.2	242.5	243.1	246.1	249.5	253.3

Name: Triethylgallium
Formula: $C_6H_{15}Ga$

CAS–RN: 1115–99–7
Group No.: 73–021
Molar Mass: 156.91

TABLE 73.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
72MAS/FAM	200.0–300.0	12S	0.40	99.	chrom	C_p	BSAO	56POP/KOL

TABLE 73.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	12	12	0.276	3.46–2	0.11	4.88–5	–2
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
200.0–300.0		4.10469	2.97868+1	–1.26294+1	1.99049		III

TABLE 73.21.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.541	1.558	1.574	1.591	1.609	1.629	1.651
C_p (J K^{-1}mol^{-1})	241.8	244.4	247.0	249.6	252.5	255.6	259.1
Temp. (K)	270	273.15	280	290	298.15	300	
c_p (J K^{-1}g^{-1})	1.677	1.685	1.706	1.739	1.770	1.777	
C_p (J K^{-1}mol^{-1})	263.1	264.4	267.6	272.9	277.7	278.9	

Name: Triethylindium
Formula: $C_6H_{15}In$

CAS–RN: 923–34–2
Group No.: 73–022
Molar Mass: 202.01

TABLE 73.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73MAS/NOV	240.0–298.1	7S	0.50	99.2	melpt	C_p	BSAO	66NIK/LEB

TABLE 73.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	7	7	0.059	1.05–2	0.03	–4.90–6	1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
240.0–298.1		–7.71331+1	1.21614+2	–4.36121+1	5.20621		IV

TABLE 73.22.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p (J K^{-1}g^{-1})	1.461	1.468	1.471	1.472	1.472	1.472	1.471
C_p (J K^{-1}mol^{-1})	295.2	296.6	297.2	297.4	297.4	297.3	297.2
Temp. (K)	298.15	300					
c_p (J K^{-1}g^{-1})	1.472	1.472					
C_p (J K^{-1}mol^{-1})	297.3	297.4					

Name: Triethylstibine
Formula: $C_6H_{15}Sb$

CAS–RN: 617–85–6
Group No.: 73–023
Molar Mass: 208.94

TABLE 73.23.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73MAS/NOV	160.0–298.1	15S	0.50	97.2	melpt	C_p	BSAO	66NIK/LEB

TABLE 73.23.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	15	15	0.163	2.19–2	0.08	2.66–5	–1
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
160.0–298.1		3.23245+1	–9.24869	3.94070	–4.01786–1		IV

TABLE 73.23.4. Recommended values of heat capacities

Temp. (K)	160	170	180	190	200	210	220
c_p (J K^{-1}g^{-1})	1.033	1.035	1.039	1.043	1.050	1.057	1.065
C_p (J K^{-1}mol^{-1})	215.9	216.3	217.0	218.0	219.3	220.8	222.6
Temp. (K)	230	240	250	260	270	273.15	280
c_p (J K^{-1}g^{-1})	1.075	1.085	1.097	1.108	1.121	1.125	1.134
C_p (J K^{-1}mol^{-1})	224.6	226.8	229.1	231.6	234.2	235.1	237.0
Temp. (K)	290	298.15	300				
c_p (J K^{-1}g^{-1})	1.148	1.159	1.162				
C_p (J K^{-1}mol^{-1})	239.8	242.2	242.8				

Name: Tetraethylgermane
Formula: $C_8H_{20}Ge$

CAS-RN: 597-63-7
Group No.: 73-024
Molar Mass: 188.86

TABLE 73.24.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54STA/WAR		190.0–220.0	4S	1.00	99.89	melpt	C_p	BSAO	49STA/GUP
72MAS/RAB		190.0–300.0	13S	0.40	99.3	melpt	C_p	BSAO	56POP/KOL
85RAB/SHE	N	181.0–307.7	33	0.30	99.45	melpt	C_p	BSAO	85RAB/SHE

85RAB/SHE misprint in the source: 268.21 K should read 263.21 K

TABLE 73.24.2. Correlated heat capacities

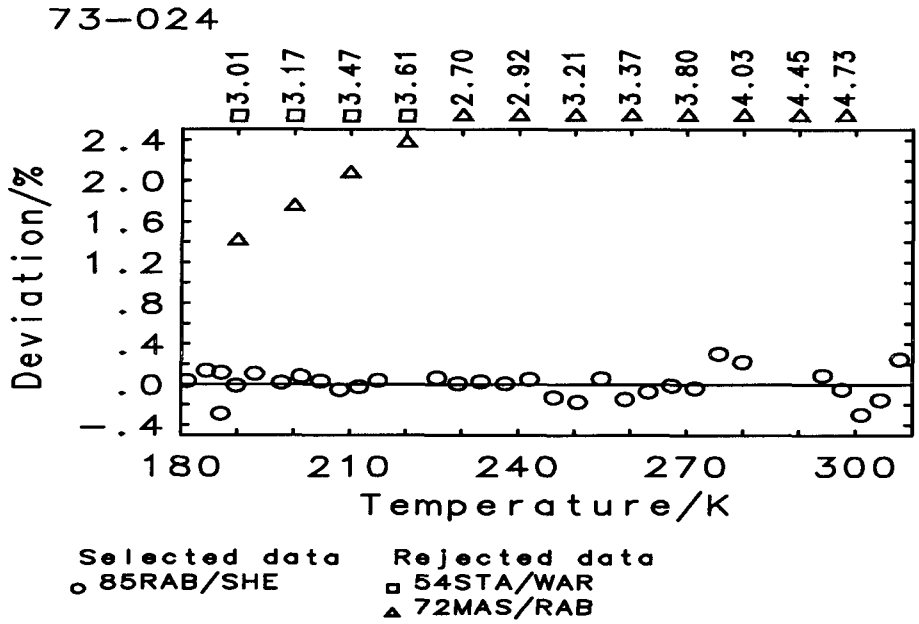
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
85RAB/SHE	181.0–307.7	32	0.30	0.444	4.53–2	0.13	1.20–4	2
				Rejected data				
54STA/WAR	(1.10, 3.32, 1.10, 4)			72MAS/RAB	(1.21, 3.38, 1.13, 13)			

TABLE 73.24.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	50	32	0.475	4.84–2	0.14	1.20–4	2
Temp. range K	A_1	A_2	A_3	A_4			Level of uncertainty
181.0–307.7	2.09648+1	1.08542+1	–4.07756	6.94114–1			III

TABLE 73.24.4. Recommended values of heat capacities

Temp. (K)	180	190	200	210	220	230	240
c_p (J K^{-1}g^{-1})	1.380	1.392	1.405	1.418	1.431	1.444	1.458
C_p (J K^{-1}mol^{-1})	260.6	263.0	265.4	267.8	270.2	272.8	275.4
Temp. (K)	250	260	270	273.15	280	290	298.15
c_p (J K^{-1}g^{-1})	1.473	1.489	1.506	1.512	1.524	1.544	1.562
C_p (J K^{-1}mol^{-1})	278.2	281.2	284.4	285.5	287.9	291.7	295.0
Temp. (K)	300	310					
c_p (J K^{-1}g^{-1})	1.566	1.590					
C_p (J K^{-1}mol^{-1})	295.8	300.2					



Name: Tetraethylplumbane
Formula: $C_8H_{20}Pb$

CAS-RN: 78-00-2
Group No.: 73-025
Molar Mass: 323.45

TABLE 73.25.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54STA/WAR	150.0	1	1.00	99.92	melpt	C_p	BSAO	49STA/GUP
56SCO/GOO	298.1	1	nosp	99.9	estim	C_p	BSAO	43RUE/HUF
89RAB/NIS1	141.6–313.8	58	0.20	99.958	melpt	C_p	BSAO	85RAB/SHE

TABLE 73.25.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
89RAB/NIS1	143.8–313.8	57	0.20	0.660	4.56-2	0.13	1.17-4	8
				Rejected data				
54STA/WAR	(1.32-1, 0.42, 1.32-1, 1)			56SCO/GOO	(2.96-1, 0.79, 2.96-1, 1)			

TABLE 73.25.3. Parameters of regression polynomial

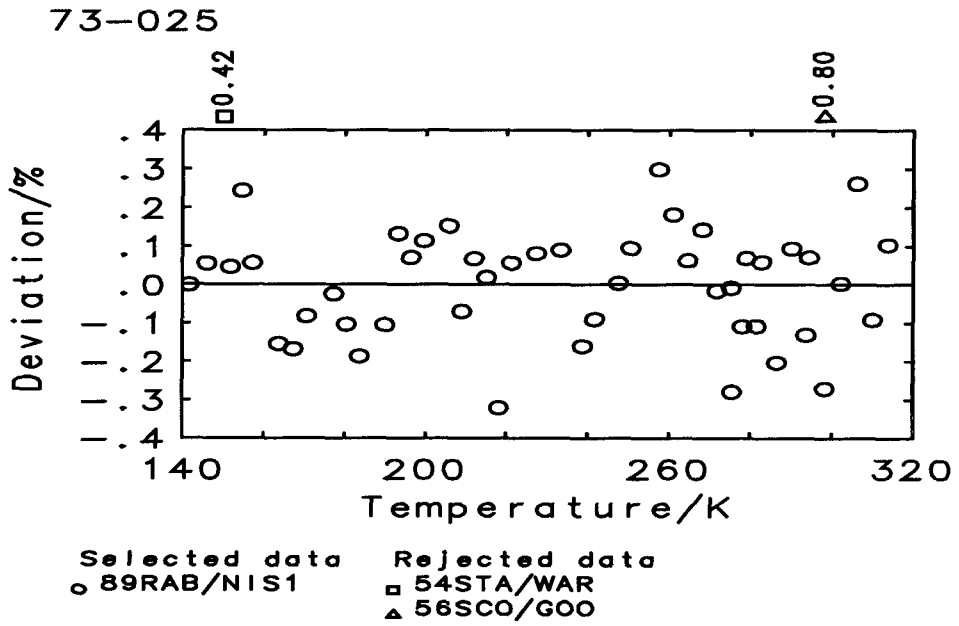
Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	60	57	0.678	4.68–2	0.14	1.17–4	8
Temp. range K		A_1	A_2	A_3			Level of uncertainty
143.8–313.8		2.94870+1	–8.63701–2	8.71580–1			II

TABLE 73.25.4. Recommended values of heat capacities

Temp. (K)	140	150	160	170	180	190	200
c_p ($J K^{-1} g^{-1}$)	0.799	0.805	0.812	0.819	0.827	0.835	0.843
C_p ($J K^{-1} mol^{-1}$)	258.4	260.4	262.6	264.9	267.4	270.0	272.7
Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1} g^{-1}$)	0.852	0.862	0.871	0.882	0.892	0.904	0.915
C_p ($J K^{-1} mol^{-1}$)	275.6	278.7	281.9	285.2	288.7	292.3	296.1
Temp. (K)	273.15	280	290	298.15	300	310	
c_p ($J K^{-1} g^{-1}$)	0.919	0.927	0.940	0.951	0.953	0.966	
C_p ($J K^{-1} mol^{-1}$)	297.3	300.0	304.0	307.4	308.2	312.6	

TABLE 73.25.5. Parameters of quasi-polynomial equation

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	60	57	0.760	5.19–2	0.15	1.43–4	10
Temp. range K	T_c K	A_1	A_2	A_3	A_4		Level of uncertainty
143.8–313.8	712.00	3.40969	1.47357+1	1.33992+1	1.97242–1		II



Name: Tetraethylstannane
Formula: $C_8H_{20}Sn$

CAS–RN: 597–64–8
Group No.: 73–026
Molar Mass: 234.96

TABLE 73.26.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
54STA/WAR	150.0–210.0	7S	1.00	99.92	melpt	C_p	BSAO	49STA/GUP
72MAS/RAB	150.0–300.0	17S	0.40	99.6	melpt	C_p	BSAO	56POP/KOL

TABLE 73.26.2. Correlated heat capacities

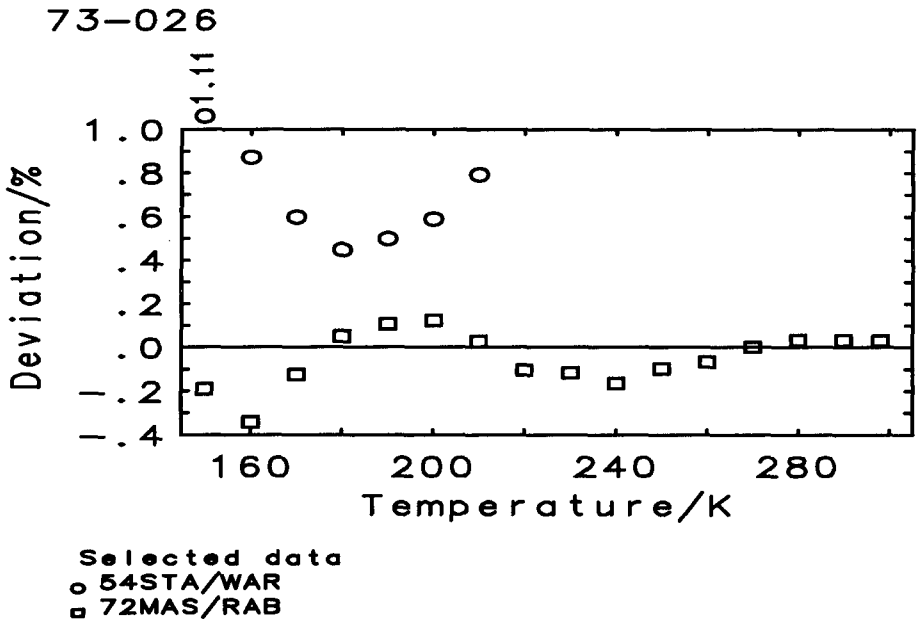
Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/–
				Selected data				
54STA/WAR	150.0–210.0	7	1.00	0.732	2.32–1	0.73	2.22–1	7
72MAS/RAB	150.0–300.0	17	0.40	0.318	4.04–2	0.13	–1.43–2	0

TABLE 73.26.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	24	24	0.510	1.39–1	0.44	5.45–2	7
Temp. range K		A_1	A_2	A_3			Level of uncertainty
150.0–300.0		2.75708+1	1.14859	5.93586–1			III

TABLE 73.26.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p ($J\,K^{-1}g^{-1}$)	1.084	1.094	1.105	1.117	1.129	1.141	1.154
C_p ($J\,K^{-1}mol^{-1}$)	254.7	257.2	259.7	262.4	265.2	268.1	271.1
Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J\,K^{-1}g^{-1}$)	1.167	1.180	1.194	1.209	1.223	1.239	1.243
C_p ($J\,K^{-1}mol^{-1}$)	274.1	277.3	280.6	284.0	287.4	291.0	292.1
Temp. (K)	280	290	298.15	300			
c_p ($J\,K^{-1}g^{-1}$)	1.254	1.270	1.284	1.287			
C_p ($J\,K^{-1}mol^{-1}$)	294.7	298.4	301.6	302.3			



Name: Tripropylaluminium
Formula: $C_9H_{21}Al$

CAS–RN: 102–67–0
Group No.: 73–027
Molar Mass: 156.25

TABLE 73.27.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
84SHE/NIS	150.0–298.1	4S	0.20	99.9	chrom	C_p	BSAO	80GUR/GAV

TABLE 73.27.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	4	4	0.000	0.00	0.00	3.34–6	0
Temp. range K		A_1	A_2	A_3	A_4		Level of uncertainty
150.0–298.1		–5.69471–1	3.83151+1	–1.59033+1	2.59042		III

TABLE 73.27.4. Recommended values of heat capacities

Temp. (K)	150	160	170	180	190	200	210
c_p ($J K^{-1}g^{-1}$)	1.589	1.630	1.667	1.702	1.734	1.765	1.796
C_p ($J K^{-1}mol^{-1}$)	248.3	254.7	260.5	265.9	270.9	275.8	280.6
Temp. (K)	220	230	240	250	260	270	273.15
c_p ($J K^{-1}g^{-1}$)	1.827	1.860	1.894	1.932	1.973	2.019	2.034
C_p ($J K^{-1}mol^{-1}$)	285.5	290.5	295.9	301.8	308.2	315.4	317.8
Temp. (K)	280	290	298.15	300			
c_p ($J K^{-1}g^{-1}$)	2.070	2.127	2.179	2.192			
C_p ($J K^{-1}mol^{-1}$)	323.4	332.4	340.5	342.5			

Name: Ferrocene
Formula: $C_{10}H_{10}Fe$

CAS-RN: 102-54-5
Group No.: 73-028
Molar Mass: 186.04

TABLE 73.28.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
69JOE/GJA	N	448.0–485.0	2	3.00	not specified		C_p	DSIO	38FRE/HIL1

69JOE/GJA constant value calculated from temperature dependence of enthalpy by the authors

TABLE 73.28.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
448.0–485.0		3.93012+1					VI

TABLE 73.28.4. Recommended values of heat capacities

Temp. (K)	450	460	470	480	490
c_p ($J K^{-1}g^{-1}$)	1.76	1.76	1.76	1.76	1.76
C_p ($J K^{-1}mol^{-1}$)	327	327	327	327	327

Name: Diphenylgermane
Formula: $C_{12}H_{12}Ge$

CAS-RN: 1675-58-7
Group No.: 73-029
Molar Mass: 228.84

TABLE 73.29.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79LEB/LEB1	239.4–330.0	5S	0.20	99.0	melpt	C_p	BSAO	76LEB/LIT

TABLE 73.29.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	5	5	0.582	3.76–2	0.12	4.23–5	–1

Temp. range K	A_1	A_2	A_3	Level of uncertainty
239.4–330.0	3.47133+1	–6.20045	2.06331	III

TABLE 73.29.4. Recommended values of heat capacities

Temp. (K)	240	250	260	270	273.15	280	290
c_p ($J K^{-1}g^{-1}$)	1.152	1.167	1.182	1.200	1.205	1.218	1.238
C_p ($J K^{-1}mol^{-1}$)	263.7	267.0	270.6	274.5	275.8	278.8	283.4
Temp. (K)	298.15	300	310	320	330		
c_p ($J K^{-1}g^{-1}$)	1.256	1.260	1.283	1.308	1.334		
C_p ($J K^{-1}mol^{-1}$)	287.4	288.4	293.7	299.3	305.3		

Name: Diethynyldiphenylgermane
Formula: $C_{16}H_{12}Ge$

CAS-RN: 1675-59-8
Group No.: 73-030
Molar Mass: 276.88

TABLE 73.30.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75LEB/MIL1	N	319.6–325.6	5	0.20	99.772	melpt	C_p	BSAO	66NIK/LEB

75LEB/MIL1 smoothed values in 75LEB/MIL2

TABLE 73.30.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	5	5	0.147	1.39–2	0.03	–3.05–5	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
319.6–325.6	–3.73137+2	2.54666+2	–3.85214+1	III

TABLE 73.30.4. Recommended values of heat capacities

Temp. (K)	320	330
c_p (J K^{-1}g^{-1})	1.421	1.434
C_p (J K^{-1}mol^{-1})	393.6	397.1

Name: Tetrabutylgermane
Formula: $C_{16}H_{36}Ge$

CAS–RN: 1067–42–1
Group No.: 73–031
Molar Mass: 301.07

TABLE 73.31.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
71SHA/YAK	N	198.6–298.1	3S	nosp	99.6	chrom	C_p	not specified	

71SHA/YAK measured data deposited in VINITI (document number unspecified)

TABLE 73.31.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	3	3	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	A_2	A_3	Level of uncertainty
198.6–298.1	4.61161+1	4.42798	4.31486–1	V

TABLE 73.31.4. Recommended values of heat capacities

Temp. (K)	200	210	220	230	240	250	260
c_p (J K^{-1}g^{-1})	1.57	1.58	1.60	1.62	1.64	1.65	1.67
C_p (J K^{-1}mol^{-1})	471	477	482	487	492	498	503

Temp. (K)	270	273.15	280	290	298.15	300
c_p (J K^{-1}g^{-1})	1.69	1.70	1.71	1.73	1.74	1.75
C_p (J K^{-1}mol^{-1})	509	511	515	520	525	526

Name: Tetrapentylstannane
Formula: $C_{20}H_{44}Sn$

CAS–RN: 3765–65–9
Group No.: 73–032
Molar Mass: 403.28

TABLE 73.32.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
72MAS/RAB	210.0–300.0	11S	0.40	98.3	melpt	C_p	BSAO	56POP/KOL

TABLE 73.32.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	11	11	0.690	1.97–1	0.28	7.75–4	0
Temp. range K		A_1	A_2	A_3			Level of uncertainty
210.0–300.0		6.04456+1	3.42311–1	1.92095			IV

TABLE 73.32.4. Recommended values of heat capacities

Temp. (K)	210	220	230	240	250	260	270
c_p ($J K^{-1} g^{-1}$)	1.436	1.453	1.472	1.491	1.511	1.532	1.554
C_p ($J K^{-1} mol^{-1}$)	579.0	586.1	593.6	601.4	609.5	617.9	626.7
Temp. (K)	273.15	280	290	298.15	300		
c_p ($J K^{-1} g^{-1}$)	1.561	1.576	1.600	1.619	1.624		
C_p ($J K^{-1} mol^{-1}$)	629.5	635.8	645.2	653.0	654.9		

74. Salts of Organic Acids

This family contains 21 salts of organic acids and one salt of 1-butanol; four compounds were measured at one temperature only. For 15 compounds, data are available at two temperatures only.

The main criterion for inclusion of a compound in the database was the melting temperature below 573 K; since most salts have high melting temperatures a good part of experimental data available is not within the scope of this publication. Most investigations on liquid salts were performed over a narrow temperature range only such as measurements from UMAA for sodium formate (83FRA/WES) for an interval of only 8 K, or the reliable measurements of heat capacity of liquid tetrahexylammonium perchlorate from KSUK (73AND/GOR) only over an interval of 2 K. Regarding the temperature range, the data for sodium butanoate (75FER/FRA) obtained on a commercial DSC calorimeter are exceptional because they are available over an interval of 50 K. However, we have assigned the level of uncertainty VI to the recommended values for this compound in a manner similar to the data for sodium formate studied in the same laboratory. A comparison of data (75FER/SAN) with reliable values from UMAA (83FRA/WES) showed that the uncertainty of the former data is much lower than that claimed in the former source.

Data for 13 compounds were measured at the University of Ile-Ife, Nigeria (76ADE/SIM, 78ADE), but data at just two temperatures are available for each compound. The heat capacities obtained using a Mettler DSC are identical at the two reported temperatures. This is highly suspicious as for some compounds the temperature range is as large as 80 K. We have no explanation to justify this finding.

Two values of the average heat capacity for the titanium (4+) salt of 1-butanol were obtained at 353 K and 443 K in a fSU laboratory (79SAM/GRI). The two values differ more than expected and the heat capacity related to the lower temperature is higher than that related to the upper temperature. For that reason, the source is cited in the table of Experimental Heat Capacities but no recommended values have been generated.

Name: Sodium salt formic acid
Formula: $CHNaO_2$

CAS-RN: 141-53-7
Group No.: 74-001
Molar Mass: 68.01

TABLE 74.1.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75FER/SAN	550.0–560.0	2	3.00	not specified		C_p	BDHT	69PER/COM
83FRA/WES	564.5–579.2	6	nosp	not specified		C_p	BSAO	68WES/WES

TABLE 74.1.2. Correlated heat capacities

Reference	Temp. range K	No. pnts used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/-
				Selected data				
83FRA/WES	564.5–579.2	6	0.30#	0.221	1.75–2	0.07	2.35–5	0

TABLE 74.1.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	8	6	0.271	2.14–2	0.08	2.35–5	0

Temp. range K	A_1	A_2	Level of uncertainty
564.5–579.2	1.70576+1	1.63041	III

TABLE 74.1.4. Recommended values of heat capacities

Temp. (K)	565	570	575	580
c_p ($J\,K^{-1}g^{-1}$)	3.212	3.222	3.232	3.242
C_p ($J\,K^{-1}mol^{-1}$)	218.4	219.1	219.8	220.5

Name: Sodium salt propanoic acid
Formula: $C_3H_5NaO_2$

CAS–RN: 137–40–6
Group No.: 74–002
Molar Mass: 96.06

TABLE 74.2.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75FER/SAN	570.0–580.0	2	3.00	not specified		C_p	BDHT	69PER/COM

TABLE 74.2.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	–9.54–7	0

Temp. range K	A_1	A_2	Level of uncertainty
570.0–580.0	2.15377+1	1.00643	VI

TABLE 74.2.4. Recommended values of heat capacities

Temp. (K)	570	580
c_p ($J\,K^{-1}g^{-1}$)	2.36	2.37
C_p ($J\,K^{-1}mol^{-1}$)	227	228

Name: Sodium salt butanoic acid
Formula: $C_4H_7NaO_2$

CAS–RN: 156–54–7
Group No.: 74–003
Molar Mass: 110.09

TABLE 74.3.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
75FER/FRA	540.0–590.0	6S	1.10	not specified		C_p	BDHT	69PER/COM

TABLE 74.3.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	6	6	0.847	8.26–1	2.54	2.83–2	4
Temp. range K		A_1	A_2				Level of uncertainty
540.0–590.0		1.46363+1	3.37036				VI

TABLE 74.3.4. Recommended values of heat capacities

Temp. (K)	540	550	560	570	580	590
c_p ($J K^{-1}g^{-1}$)	2.48	2.51	2.53	2.56	2.58	2.61
C_p ($J K^{-1}mol^{-1}$)	273	276	279	281	284	287

Name: Lead(2+) salt hexanoic acid
Formula: $C_{12}H_{22}O_4Pb$

CAS-RN: 15773-53-2
Group No.: 74-004
Molar Mass: 437.50

TABLE 74.4.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76ADE/SIM	413.0–493.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.4.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
413.0–493.0		7.24035+1					VI

TABLE 74.4.4. Recommended values of heat capacities

Temp. (K)	410	430	450	470	490
c_p ($J K^{-1}g^{-1}$)	1.38	1.38	1.38	1.38	1.38
C_p ($J K^{-1}mol^{-1}$)	602	602	602	602	602

Name: Mercury(2+) salt octanoic acid
Formula: $C_{16}H_{30}HgO_4$

CAS–RN: 28043–54–1
Group No.: 74–005
Molar Mass: 487.00

TABLE 74.5.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78ADE	400.0–425.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.5.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
400.0–425.0	7.64326+1	VI

TABLE 74.5.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430
c_p ($J\,K^{-1}g^{-1}$)	1.30	1.30	1.30	1.30
C_p ($J\,K^{-1}mol^{-1}$)	636	636	636	636

Name: Lead(2+) salt octanoic acid
Formula: $C_{16}H_{30}O_4Pb$

CAS–RN: 7319–86–0
Group No.: 74–006
Molar Mass: 493.61

TABLE 74.6.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76ADE/SIM	413.0–493.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.6.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–493.0	9.21281+1	VI

TABLE 74.6.4. Recommended values of heat capacities

Temp. (K)	410	430	450	470	490
c_p ($J\,K^{-1}g^{-1}$)	1.55	1.55	1.55	1.55	1.55
C_p ($J\,K^{-1}mol^{-1}$)	766	766	766	766	766

Name: Titanium(4+) salt 1–butanol
Formula: $C_{16}H_{36}O_4Ti$

CAS–RN: 5593–70–4
Group No.: 74–007
Molar Mass: 340.34

TABLE 74.7.1. Experimental heat capacities

Reference		Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
79SAM/GRI	N	353.1–443.1	2	nosp	99.95	chrom	C_{avg}	not specified	

79SAM/GRI average values in temperature ranges 333–373 K and 433–453 K; substance associated forming dimer below 393 K

Name: Mercury(2+) salt decanoic acid
Formula: $C_{20}H_{38}HgO_4$

CAS–RN: 27394–49–6
Group No.: 74–008
Molar Mass: 543.11

TABLE 74.8.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78ADE	403.0–420.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.8.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
403.0–420.0		9.82619+1					VI

TABLE 74.8.4. Recommended values of heat capacities

Temp. (K)	400	410	420
c_p ($J\,K^{-1}g^{-1}$)	1.50	1.50	1.50
C_p ($J\,K^{-1}mol^{-1}$)	817	817	817

Name: Lead(2+) salt decanoic acid
Formula: $C_{20}H_{38}PbO_4$

CAS–RN: 15773–52–1
Group No.: 74–009
Molar Mass: 549.72

TABLE 74.9.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76ADE/SIM	413.0–453.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.9.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
413.0–453.0		1.00667+2					VI

TABLE 74.9.4. Recommended values of heat capacities

Temp. (K)	410	430	450
c_p ($J K^{-1} g^{-1}$)	1.52	1.52	1.52
C_p ($J K^{-1} mol^{-1}$)	837	837	837

Name: Cadmium salt dodecanoic acid
Formula: $C_{24}H_{46}CdO_4$

CAS–RN: 2605–44–9
Group No.: 74–010
Molar Mass: 511.04

TABLE 74.10.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78KON/RUF	N	400.00	1.779	6.00	not specified		C_p	BDHT	76MET/COM

78KON/RUF temperature not specified; estimated according to other data by the same authors

Name: Mercury(2+) salt dodecanoic acid
Formula: $C_{24}H_{46}HgO_4$

CAS–RN: 23186–25–6
Group No.: 74–011
Molar Mass: 599.22

TABLE 74.11.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78ADE	413.0–430.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.11.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
413.0–430.0		1.31000+2					VI

TABLE 74.11.4. Recommended values of heat capacities

Temp. (K)	410	420	430
c_p ($J\,K^{-1}g^{-1}$)	1.82	1.82	1.82
C_p ($J\,K^{-1}mol^{-1}$)	1090	1090	1090

Name: Lead(2+) salt dodecanoic acid
Formula: $C_{24}H_{46}O_4Pb$

CAS–RN: 15773–55–4
Group No.: 74–012
Molar Mass: 605.83

TABLE 74.12.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76ADE/SIM	413.0–473.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.12.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–473.0	1.29893+2	VI

TABLE 74.12.4. Recommended values of heat capacities

Temp. (K)	410	440	470
c_p ($J\,K^{-1}g^{-1}$)	1.78	1.78	1.78
C_p ($J\,K^{-1}mol^{-1}$)	1080	1080	1080

Name: *N,N,N*–Trihexyl–1–hexanaminium perchlorate
Formula: $C_{24}H_{52}ClNO_4$

CAS–RN: 4656–81–9
Group No.: 74–013
Molar Mass: 454.13

TABLE 74.13.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
73AND/GOR	380.5–386.6	6	nosp	99.94	melpt	C_p	BSAO	53WES/HAT

TABLE 74.13.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	6	6	0.084	2.99–2	0.03	1.02–5	–1
Temp. range K		A_1	A_2				Level of uncertainty
380.5–386.6		5.09693+1	1.77836+1				III

TABLE 74.13.4. Recommended values of heat capacities

Temp. (K)	380	390
c_p ($J K^{-1} g^{-1}$)	2.170	2.203
C_p ($J K^{-1} mol^{-1}$)	985.7	1000

Name: Cadmium salt tetradecanoic acid
Formula: $C_{28}H_{54}CdO_4$

CAS–RN: 10196–67–5
Group No.: 74–014
Molar Mass: 567.15

TABLE 74.14.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78KON/RUF	N	410.00	2.151	2.50	not specified		C_p	BDHT	76MET/COM

78KON/RUF temperature not specified; estimated according to other data by the same authors

Name: Mercury(2+) salt tetradecanoic acid
Formula: $C_{28}H_{54}HgO_4$

CAS–RN: 36215–49–3
Group No.: 74–015
Molar Mass: 655.32

TABLE 74.15.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78ADE	413.0–421.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.15.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
413.0–421.0		1.36568+2					VI

TABLE 74.15.4. Recommended values of heat capacities

Temp. (K)	410	420
c_p ($J K^{-1} g^{-1}$)	1.73	1.73
C_p ($J K^{-1} mol^{-1}$)	1140	1140

Name: Lead(2+) salt tetradecanoic acid
Formula: $C_{28}H_{54}O_4Pb$

CAS-RN: 32112-52-0
Group No.: 74-016
Molar Mass: 661.93

TABLE 74.16.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76ADE/SIM	413.0–473.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.16.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–473.0	1.58759+2	VI

TABLE 74.16.4. Recommended values of heat capacities

Temp. (K)	410	430	450	470
c_p ($J K^{-1} g^{-1}$)	1.99	1.99	1.99	1.99
C_p ($J K^{-1} mol^{-1}$)	1320	1320	1320	1320

Name: Cadmium salt hexadecanoic acid
Formula: $C_{32}H_{62}CdO_4$

CAS-RN: 6427-86-7
Group No.: 74-017
Molar Mass: 623.25

TABLE 74.17.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78KON/RUF	N	430.00	2.246	2.00	not specified		C_p	BDHT	76MET/COM

78KON/RUF temperature not specified; estimated according to other data by the same authors

Name: Mercury(2+) salt hexadecanoic acid
Formula: $C_{32}H_{62}HgO_4$

CAS–RN: 16888–60–1
Group No.: 74–018
Molar Mass: 711.43

TABLE 74.18.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
78ADE	396.0–421.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.18.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
396.0–421.0	1.46407+2	VI

TABLE 74.18.4. Recommended values of heat capacities

Temp. (K)	400	410	420
c_p ($J\,K^{-1}g^{-1}$)	1.71	1.71	1.71
C_p ($J\,K^{-1}mol^{-1}$)	1220	1220	1220

Name: Lead(2+) salt hexadecanoic acid
Formula: $C_{32}H_{62}O_4Pb$

CAS–RN: 15773–56–5
Group No.: 74–019
Molar Mass: 718.04

TABLE 74.19.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	Purity method	Type capacity	Calorimeter Type	Calorimeter Reference
76ADE/SIM	413.0–473.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.19.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
413.0–473.0	1.70786+2	VI

TABLE 74.19.4. Recommended values of heat capacities

Temp. (K)	410	430	450	470
c_p ($J\,K^{-1}g^{-1}$)	1.98	1.98	1.98	1.98
C_p ($J\,K^{-1}mol^{-1}$)	1420	1420	1420	1420

Name: Cadmium salt octadecanoic acid
Formula: $C_{36}H_{70}CdO_4$

CAS-RN: 2223-93-0
Group No.: 74-020
Molar Mass: 679.36

TABLE 74.20.1. Experimental heat capacities

Reference		Temp. K	Capac. J/(K.g)	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78KON/RUF	N	420.00	2.208	2.00	not specified		C_p	BDHT	76MET/COM

78KON/RUF temperature not specified; estimated according to other data by the same authors

Name: Mercury(2+) salt octadecanoic acid
Formula: $C_{36}H_{70}HgO_4$

CAS-RN: 645-99-8
Group No.: 74-021
Molar Mass: 767.54

TABLE 74.21.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
78ADE	391.0–433.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.21.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/-
C_p	2	2	0.000	0.00	0.00	0.00	0

Temp. range K	A_1	Level of uncertainty
391.0–433.0	1.65638+2	VI

TABLE 74.21.4. Recommended values of heat capacities

Temp. (K)	400	410	420	430
c_p ($J K^{-1}g^{-1}$)	1.79	1.79	1.79	1.79
C_p ($J K^{-1}mol^{-1}$)	1380	1380	1380	1380

Name: Lead(2+) salt octadecanoic acid
Formula: $C_{36}H_{70}O_4Pb$

CAS-RN: 1072-35-1
Group No.: 74-022
Molar Mass: 774.15

TABLE 74.22.1. Experimental heat capacities

Reference	Temp. range K	No. pnts	Error %	Purity %	method	Type capacity	Calorimeter Type	Reference
76ADE/SIM	413.0–453.0	2	2.00	not specified		C_p	BDHT	76MET/COM

TABLE 74.22.3. Parameters of regression polynomial

Heat capacity type	No. data points total	used	s_w	s/R	s_r %	s_b/R	+/–
C_p	2	2	0.000	0.00	0.00	0.00	0
Temp. range K		A_1					Level of uncertainty
413.0–453.0		1.73191+2					VI

TABLE 74.22.4. Recommended values of heat capacities

Temp. (K)	410	420	430	440	450
c_p ($J K^{-1} g^{-1}$)	1.86	1.86	1.86	1.86	1.86
C_p ($J K^{-1} mol^{-1}$)	1440	1440	1440	1440	1440