Heat Capacities of Organic Compounds in Liquid State II. C_1 to C_{18} n-Alkanes

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(Received 29 January 1990; accepted 24 July 1990)

Heat capacities of liquid C_1 to C_{18} n-alkanes measured by calorimetric methods have been compiled and 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 presented. Heat capacities were also fitted by a quasipolynomial equation permitting extrapolation of heat capacities outside the temperature range of experimental values.

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1. Introduction

This article is the second part of a communication on heat capacities of important organic compounds in liquid state. The main objective of this work was to review and evaluate all available calorimetric data on liquid heat capacities of n-alkanes up to C_{18} and to present the "best" recommended values obtained by temperature correlation of the data from the selected sources.

The Subcommittee on Thermodynamic Data of the IUPAC Commission on Thermodynamics has been encouraging international projects aimed at the establishment of evaluated thermodynamic data. This article was prepared in direct connection with the IUPAC projects "The Vapor-Liquid Equilibria in 1-Alkanol + n-Alkanes Mixtures" and "The Heat Capacities of Liquid Substances".

The first part of this communication (90ZAB/RUZ2) contained the review, evaluation, and temperature correlation of the heat capacities for liquid C_1 to C_{18} 1-alkanols. This part deals in an analogous way with the data for n-alkanes. As both articles have the same structure and the procedure was described thoroughly in the previous part we only briefly recapitulate the main features, and repeat most of the definitions and table descriptions. The reader should be able to use this article without consulting the previous one which is, however, recommended to those who would like to have a deeper insight into the methodology of evaluating and correlating the data.

1.1. Previous compilations

There are not many compilations which review heat capacities of liquid n-alkanes. From older sources the most important is the compilation of Makita and Touloukian

(70TOU/MAK) which gives recommended values for C_1 to C_{10} n-alkanes. Several important measurements were performed since then, especially for lower n-alkanes. The Supplement to the above compilation (76TOU/MAK) lists some of the newer results and contains values for the higher n-alkanes. However, only raw data are presented and the Supplement lacks any evaluation.

A number of heat capacity sources for n-alkanes is summarized in the compilation of thermodynamic properties by Domalski *et al.* (84DOM/EVA). However, the data are given at one temperature only and no recommended data are presented.

Some recommended values for heat capacities were also published in the specialized literature which is not generally available. Tables published by the Engineering Science Data Unit (77ENG) contain temperature correlations of recommended data for C_1 to C_{14} n-alkanes; the continuously updated tables published at the Thermodynamics Research Center of Texas A&M University (87TRC) give recommended values for C_6 to C_{10} n-alkanes. The Design Institute for Physical Property Data (DIPPR) released recently parameters for a polynomial representing the evaluated data for C_1 to C_{16} n-alkanes (85DIP). As this data base is widely used we made a comparison with our recommendations (see Sec. 4.7 in Table 56).

Several general tables of physico-chemical properties list also heat capacities for n-alkanes (see Ref. 85WIL/CHA for listing of the most important).

1.2. Types of heat capacity data

Two types of heat capacities are encountered throughout this article. The isobaric heat capacity determined by measurements at constant pressure is defined as

$$C_p^l = T\cdot(\partial S^l/\partial T)_p = (\partial H^l/\partial T)_p. \quad (1)$$

The saturation heat capacity results from measurements carried out under conditions of vapor-liquid equilibrium and is defined as

$$C_{sat}^l = T\cdot(\partial S^l/\partial T)_{sat}, \quad (2)$$

where the subscript sat denotes that pressure changes with temperature along the vapor-liquid saturation curve. Values obtained from calorimetric experiments correspond to a finite temperature change and cannot be automatically considered as C_p^l and C_{sat}^l defined by Eqs. (1) and (2). In those cases where the temperature step in the experiment exceeded 10 K, the value obtained is denoted in the tables of experimental values as the average heat capacity C_{avg}^l. This type of quantity has never been used for establishing the recommended values.

The equation connecting C_{sat}^l and C_p^l at the same temperature T and vapor pressure p_{sat} is:

$$C_{sat}^l = C_p^l - T\cdot(\partial V^l/\partial T)_p\cdot(dp/dT)_{sat}. \quad (3)$$

The conversion can be made from the temperature dependence of the liquid density and vapor pressure. The correction term plays a role only at temperature above the normal boiling point temperature T_b. Below that temperature its magnitude is less than 0.1 percent of heat capacity value.

Isobaric heat capacity is practically pressure independent below T_b and 0.1 MPa; the recommended C_p^l tabulated in this article above the normal boiling temperature are values of the vapor pressure of the compound. The experimental results determined at pressures remote from the vapor pressure were considered (after the appropriate correction) in those cases when they extended the temperature range of available data.

Both C_p^l and C_{sat}^l are tabulated for those compounds where the difference between the two is not substantially smaller than the uncertainty of experimental data in some part of the temperature range. Appropriate conversions between C_p^l and C_{sat}^l were carried out first and then both types of heat capacity data were correlated separately. The same data sources were used for calculating the conversion term in Eq. (3) as in the previous part (90ZAB/RUZ2). The symbol C^l without a subscript specification or the term heat capacity are used throughout this paper whenever we refer both to C_p^l and C_{sat}^l or when the difference between their values for particular conditions is negligible compared to the expected experimental uncertainty.

2. Methodology of Establishing the Recommended Data

2.1. Evaluation and selection process

Experimental heat capacities of n-alkanes along with auxiliary data were stored in the database of raw data. The correlation was performed using the weighted least-squares method; the minimized objective function S had the form:

$$S = \sum_{i=1}^{n} [(C_{sm}^l - C_{exp}^l)^2/\sigma^2(C)^l]_i, \quad (4)$$

where subscript "exp" and "*sm*" relate to experimental and smoothed values, respectively. The reciprocal of the variance $\sigma^2(C^l)$ has the meaning of the weighting factor. It was estimated for each value from the assumed experimental uncertainty of the data set used in the correlation.

Selection and correlation of data for each compound was carried out simultaneously in several steps. First, a preliminary joint correlation was performed with all available data. 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. In the next step less accurate or obviously inconsistent data were tentatively discarded and possibly the weights of whole data sets were altered. The correlation was repeated several times until the final fit with the selected data was obtained. The final correlation was assigned a level of accuracy (I to VI) 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

$$s_w = [S_{min}/(n-m)]^{1/2}, \quad (5)$$

where n is the overall number of the fitted data points, m is the number of independent adjustable parameters in a correlation equation and S_{min} denotes the minimum of the function S. In addition, use of the following statistical criteria was made:

the standard deviation

$$s = \left\{ \left[\sum_{i=1}^{n} (C^l_{sm} - C^l_{\exp})_i^2 \right] / (n-m) \right\}^{1/2}, \quad (6)$$

the percentage standard deviation

$$s_r = \left\{ \left[\sum_{i=1}^{n} ((C^l_{sm} - C^l_{\exp})/C^l_{\exp})_i^2 \right] / (n-m) \right\}^{1/2} \times 100, \quad (7)$$

the bias

$$s_b = \left[\sum_{i=1}^{n} (C^l_{sm} - C^l_{\exp})_i \right] / n, \quad (8)$$

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

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

$$d_w = \left\{ \left[\sum_{i=1}^{n_1} ((C^l_{sm} - C^l_{\exp})^2/\sigma^2 C^l)_i \right] / n_1 \right\}^{1/2}, \quad (9)$$

the average deviation

$$d = \left\{ \left[\sum_{i=1}^{n_1} (C^l_{sm} - C^l_{\exp})_i^2 \right] / n_1 \right\}^{1/2}, \quad (10)$$

the average percentage deviation

$$d_r = \left\{ \left[\sum_{i=1}^{n_1} ((C^l_{sm} - C^l_{\exp}))/C^l_{\exp})_i^2 \right] / n_1 \right\}^{1/2} \cdot 100, \quad (11)$$

the bias of the data set

$$d_b = \left[\sum_{i=1}^{n_1} (C^l_{sm} - C^l_{\exp})_i \right] / n_1, \quad (12)$$

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

2.2. Correlation equations

The selected experimental values were fitted with cubic splines. In this case, the heat capacity over the whole experimental temperature range is described by $k-1$ cubic polynomials delimited by k temperatures (knots). The neighboring polynomials have at the inner limiting temperatures not only the same values of heat capacity but also identical first and second temperature derivatives. Thus there are $k+2$ independent adjustable parameters, for n-alkanes k equaled 3 to 5 depending on the width of temperature range and complexity of the heat capacity temperature dependence. A single polynomial quadratic or cubic in temperature was used for those compounds where data were available only in a limited temperature range. The tabulated adjustable parameters A_j relate to the equation

$$C^l/R = \sum_{j=0}^{m} A_j (T/100)^j, \quad (13)$$

where R is the gas constant and m equals 2 or 3.

The cubic splines are very flexible for the description of heat capacities inside the temperature range of experimental data, however, they cannot be used for a meaningful extrapolation. We described in the previous part a new "quasi-polynomial equation" which provides for a reasonable extrapolation towards the critical point.

The form

$$d(C^l/R)/d\tau = -\left(e_{-1}/\tau + \sum_{i=1}^{m_1} e_i \tau^i \right)^2, \quad (14)$$

which is always negative can be integrated to obtain

$$C^l/R = \sum_{j=-1}^{m} E_j \tau^j, \quad (15)$$

where $\tau = (1 - T/T_c)$. E_j and e_i are adjustable parameters; E_0 results from integration and other E_j's are automatically constrained by the Eq. (14) in such a way that the temperature derivative of the heat capacity must always be positive and equal infinity at the critical temperature. For most n-alkanes $m_1 = 2$ (similarly to the case of 1-alkanols), then $m = 5$ and four parameters are independent. For methane and ethane where research data reach close to the critical temperature $m_1 = 3$, then $m = 7$ and five parameters are independent.

2.3. Units, conversion factors, temperature scales

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:

$1\ \text{cal} = 4.1840\ \text{J}$
$1\ \text{Btu lb}^{-1}(\text{°F})^{-1} = 4.1868\ \text{J K}^{-1}\,\text{g}^{-1}$
$T[\text{K}] = T[\text{°C}] + 273.15$
$T[\text{K}] = T[\text{°F}] \cdot 0.555\,55 + 255.37$
$R = 8.314\,41\ \text{J K}^{-1}\,\text{mol}^{-1}$.

Molar masses were calculated from relative atomic masses recommended by the IUPAC Commission on Atomic Weights (84COM). The differences in temperature scales were neglected as discussed in Part I.

3. Heat Capacity Data on n-Alkanes—Availability, Consistency, and Temperature Dependence

The literature search was limited to sources published after 1920. Only calorimetric measurements of heat capacities were compiled. Neither enthalpic measurements on reference-fluid boil-off calorimeters nor heat capacities determined by indirect techniques (compressibility and piezothermic methods) were considered.

3.1. Selection of data for C_1 to C_4 n-alkanes

The low alkanes are gaseous at room temperature and atmospheric pressure. The amount of data is not very extensive as handling of compounds is more complicated than for higher n-alkanes. The first results were reported only in the 1920's; most of the values were determined on low temperature calorimeters.

For C_1 to C_3 n-alkanes the most important data are those obtained in the National Bureau of Standards at Boulder, Colorado on an adiabatic calorimeter with the spherical vessel described by Goodwin (61GOO). These

measurements, performed in the 1970's by Younglove, Roder, and Goodwin, cover most of the saturation line and reach close to the critical point. They were complemented by several older sources: measurements from the Technical University in Breslau, Germany for methane (29CLU), from the Cryogenic Laboratory of the Bureau of Mines at Amarillo, Texas for ethane (30WIE/HUB) and from the University of California for ethane and propane (37WIT/KEM, 38KEM/EGA). Recent results by Cutler and Morrison from the National Research Council in Ottawa on methane and propane were also included. As several consistent data sets relating to saturation conditions are available, we did not consider sources presenting values at pressures removed from the vapor pressure (79VAN/ZEL, 80MIY/HEJ).

There are much less data for butane compared with C_1 to C_3 alkanes; only four literature sources were found. Our recommended values are based on old low-temperature measurements by Aston and Messerly (40 AST/MES) from the Pennsylvania State University, complemented by the superambient data from the California Institute of Technology (35SAG/LAC). The latter source presents, however, the results only as a graph and the generation of pseudo-experimental data points is very inaccurate.

3.2. Selection of data for C_5 to C_7 n-alkanes

There are numerous data sources for C_5 to C_7 n-alkanes, especially for n-heptane which is recommended as standard substance for calibrating calorimeters.

The main contributions for pentane and hexane are low temperature measurements from the former Bureau of Mines, Bartlesville, Oklahoma (46DOU/HUF, 67MES/GUT). At superambient temperatures the results from the Groznensky Petroleum Institute (Groznenskii Neftyanoi Institut), USSR (75GRI/RAS) seem to be the most reliable. We included for both compounds another consistent Soviet source covering a wide temperature range (88MEL/VER) from the Kurskii State Pedagogical Institute (Kurskii Gosudarstvennyi Pedagogicheskii Institut). In the case of pentane we have, however, eliminated in the latter reference the data point at the highest temperature which did not correspond to the expected shape of the heat capacity curve.

The heat capacities for pentane by Peng and Stiel (74PEN/STI) were measured in the high temperature region at pressures above p_{sat}. They were not considered as any reasonable pVT formulation for liquid pentane is not available which permits conversion of thermodynamic data to the vapor pressure near the critical point. The graph by Grigor'ev *et al.* (85GRI/GER) representing measurements with pentane near the critical point was also not considered because of difficulty in interpreting the data.

In the case of hexane we included also old but reliable low-temperature measurements from the Stanford University, California (31HUF/PAR) and the extensive measurements from the Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw (80KAL/JED). Superambient values from the California Institute of Technology (51CON/SAG) were also considered as well as a number of results at room temperature obtained mostly on Picker-type calorimeters.

The position of heptane is quite special due to its frequent use as a reference material in the temperature range 0 to 400 K. The number of heat capacity values reported in the literature is enormous, however, in many cases the results are not original; the recommended data for heptane were first used for calibration, and heat capacity of heptane was then repeatedly measured to check the reproducibility of measurements. We did not, of course, include any of those values. Our recommendations are based on the measurements performed at the National Bureau of Standards, Washington D.C. (47OSB/GIN, 54DOU/FUR) and at the Bureau of Mines, Bartlesville, Oklahoma (61MCC/MES). In the case of the latter measurements we included in our fit the final critical summarization of the results as presented by Huffman *et al.* (61HUF/GRO). Three additional temperature dependent data sets, selected for the final correlation, were from the following laboratories: The University of Götingen, Germany (66KLE), The State University of Utrecht, Netherlands (79SCH/OFF) and The Polish Academy of Sciences, Warsaw (80KAL/JED). An IUPAC publication on reference materials for realization of physicochemical properties (88MAR) presents saturation heat capacities for n-heptane between 188.6 and 400 K evaluated by A. J. Head and R. Sabbah; these values are based solely on the source 54DOU/FUR. The deviations from our recommendations never exceed 0.08 percent and are in average about 0.03 percent (differences are both negative and positive).

3.3. Selection of data for C_8 to C_{18} n-alkanes

There is a limited number of literature sources reporting heat capacities for high n-alkanes (except decane) and the temperature range of measurements is not usually very large. The main basis for establishing the recommended data were measurements from the Bureau of Mines (54FIN/GRO, 67MES/GUT). For C_8 and C_9 n-alkanes several high accuracy values measured near room temperature at the National Bureau of Standards, Washington D. C. (47OSB/GIN) were also included.

Results of reasonable reliability reaching above 40 K are available only for C_8, C_{10}, C_{11}, C_{14}, and C_{16} n-alkanes. Most of the selected high temperature data were measured in the Groznensky Petroleum Institute, USSR (75GRI/RAS, 84GRI/AND, 88KUZ/KHA). For hexadecane the only high-temperature values were published by the Laboratory of Physical Chemistry, Paris (74PET/TER); two experimental data points at the highest temperature were, however, discarded in the final selection as they obviously distorted the heat capacity curve. The results from The Polytechnical Institute (Polytekhnicheskii Institut) in Baku, USSR for C_9, C_{11}, and C_{13} n-alkanes (76MUS) were entirely eliminated as their temperature variation was found completely unrealistic.

There are a number of literature sources reporting data at one temperature or in a limited temperature range near 300 K. These data were usually determined in connection with mixture investigations as the values at the limit of a

concentration range. They are in most cases largely scattered, the main reason being the low purity of samples. It does not significantly influence the excess properties of mixtures but affects strongly heat capacity of pure substances where higher accuracy is expected.

For obtaining an estimate of heat capacities at temperatures where the data are missing, the contribution method based on the recommendations in this communication (90ZAB/RUZ1) was developed.

3.4. Temperature variation of heat capacity for n-alkanes

Temperature dependence of heat capacities of liquid n-alkanes (see Figs. 18 and 19) is less complex compared to that for 1-alkanols. Accurate measurements suggest presence of a shallow minimum near the melting point of a substance; otherwise heat capacity is an increasing convex function of temperature. The curves for methane, ethane, and heptane where the data are available in the vicinity of the critical temperature demonstrate a steep increase in the heat capacity as the critical temperature is approached.

The fit of the heat capacity as a function of temperature using cubic splines was satisfactory; the deviations were within the expected error limits except for methane where the scatter was somewhat higher. For C_1, C_2, and C_7 n-alkanes where the data reach close to the critical point the total temperature range had to be divided into four subintervals in order to fit the data satisfactorily. For C_9, C_{12}, C_{13}, C_{15}, C_{17}, and C_{18} n-alkanes simple temperature polynomial of a second or third degree was sufficient to fit the data adequately.

4. Description of Tables and Deviation Plots

Most of the information on the data and their processing is given in tables described below. The characterization of raw data, their consistency, and results of correlation are summarized for each n-alkane separately in three tables (experimental heat capacities, correlated heat capacities, parameters of cubic spline or regression polynomials) and a deviation plot (Figs. 1–17). In the case of heptadecane where only one data source was considered (67MES/GUT) the table of correlated heat capacities as well as deviation plot were not produced.

At the end of the article the recommended values generated from the cubic splines or regression polynomials Eq. (13) and parameters of quasipolynomial extrapolation Eq. (15) are tabulated together for all n-alkanes in Tables 54 and 55, respectively. Graphical representation of the recommended data is in Figs. 18 and 19.

Correlations for both isobaric and saturation heat capacities were performed with cubic splines for C_1 to C_8 and C_{10} n-alkanes. No distinction is made between the two heat capacities for other compounds (see Sec. 1.2 for explanation).

The correlation with quasipolynomial equation was not carried out for tridecane and pentadecane where data were available in a too limited temperature range for considering a meaningful extrapolation. Where distinction between C^l_{sat} and C^l_p was made only the former property was correlated.

Certain statistics and parameter values are listed in the modified E notation. The first part of number denotes the fractional part which is followed by the exponent of the basis 10. The exponent is separated from the fractional part by a plus or a minus sign (e.g., $-1.53-5$ means $-1.53\cdot10^{-5}$).

4.1. 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 compound in one publication 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 are the two last digits of the year of publication, 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.

For some sources a footnote is added below the table. In these cases there is 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 "Eq." is used in those cases where only parameters of a smoothing equation were presented in the original literature, "S" denotes the cases when instead of raw values only smoothed data points were found in literature.

Fourth column: error of measurement $\sigma_r C^l_{exp}$ in percent estimated 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 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 chromatography, "estim"—the purity was estimated by the authors, "melpt"—determination of impurities from the melting point depression.

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

Seventh column: type of the calorimetric method used for determining the data and reference to the publication where the instrument is described. The abbreviations used for calorimetric techniques are as follows: AD—adiabatic calorimetry, CC—measurement of cooling curve, CT—use of the Calvet-Tian type of calorimeter, DC—differential calorimetry, DR—drop calorimetry, DS—differential scanning calorimetry, FL—flow calorimetry, IP—isoperibol calorimetry, RP—regular pulsing technique. More detailed description of individual methods can be found in (90ZAB/RUZ2).

4.2. 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.

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.

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

Fifth column: average weighted deviation d_w defined by Eq. (9).

Sixth column: average deviation d [defined by Eq. (10)] divided by gas constant R (dimensionless).

Seventh column: average percentage deviation d_r defined by Eq. (11).

Eighth column: bias of the data set d_b [defined by Eq. (12)] divided by gas constant R (dimensionless).

Ninth column: the difference between the numbers of experimental points with positive and negative deviation from the recommended values (denoted $+/-$).

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. Only the references with data inside the temperature range of the selected values are listed.

In the case of C_1 to C_8 and C_{10} n-alkanes the correlations for isobaric and saturation heat capacities were performed separately. We give, however, for these compounds only one table of correlated heat capacities as the selection of data sources did not differ and values of statistics were practically identical in both correlations.

4.3. Parameters of cubic spline polynomials

This table gives in the upper part characteristics of the final correlation of the selected data and lists in the lower part the corresponding parameters of the cubic spline polynomials.

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. Symbol C is used when it was not reasonable to make any distinction between the two types of heat capacities.

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: standard weighted deviation s_w defined by Eq. (5).

Fifth column: standard deviation s [defined by Eq. (6)] divided by gas constant R (dimensionless).

Sixth column: standard percentage deviation s_r defined by Eq. (7).

Seventh column: bias s_b [defined by Eq. (8)] divided by gas constant R (dimensionless).

Eighth column: the overall differences between the numbers of experimental points with positive and negative deviation from the recommended values (denoted $+/-$).

The parameters of polynomials describing individual subintervals of the temperature range of the selected data are listed in the lower part of the table. When both C^l_p and C^l_{sat} were correlated separately, two sets of parameters are given. 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. (13) valid in the given subinterval. Dimension of parameters is $1/T^j$.

Sixth column: level of accuracy assigned by the evaluators to the data generated from the polynomial in the given temperature subinterval. This characteristic expresses the expected overall accuracy 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 accuracy were assigned:

- I excellent data (uncertainty below 0.1 percent)
- II highly reliable data (uncertainty below 0.25 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).

4.4. 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. 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 are omitted. Some data sets that exhibit large deviations from the recommended data were not included.

4.5. Recommended values of heat capacities

Table 54 lists recommended heat capacities generated from the parameters of cubic spline polynomials at typical temperatures 273.15 and 298.15 K, and with the step 10 K over the whole temperature range of the selected experimental data.

4.6. Parameters of quasipolynomial extrapolation equation

The parameters in Table 55 represent C_p^l for C_1 to C_8 and C_{10} n-alkanes; no distinction between the types of heat capacity is made for other n-alkanes. The tabulated items have the following meaning.

First line: name of compound.

Second line: critical temperature in Kelvin.

Third to eleventh line: dimensionless parameters of Eq. (15).

Twelfth line: the standard deviation of the fit s [defined by Eq. (6)] divided by gas constant R.

Thirteenth line: level of accuracy within the temperature range of the experimental data. When using the equation outside this interval the accuracy deteriorates with the length of extrapolation.

4.7. Comparison with the DIPPR data

Table 56 summarizes results of comparisons with heat capacities in the DIPPR data base. Also the data for C_1 to C_6 1-alkanols presented in our previous communication (90ZAB/RUZ2) were considered (DIPPR data base does not cover higher members of the homologous series). The DIPPR values relate to 101.325 kPa below the normal boiling temperature and to the vapor pressure above this temperature; it is not clearly specified if the parameters represent saturation or isobaric heat capacity. We based comparison on our C_{sat} (the differences were lower compared to C_p).

The data bases which served for generating recommended data in the two projects are not comparable as DIPPR used often also secondary sources and/or extrapolated data. It can be, however, said that we have exploited some more recent references omitted in the DIPPR data base where also the Soviet sources were totally missing. Our recommendations cover wider temperature range for C_5, C_6, C_8, C_{10}, C_{11}, C_{14}, C_{16} n-alkanes and for C_4 to C_6 1-alkanols. The comparisons were performed only in the temperature intervals where both evaluations were valid.

The tabulated items have the following meaning.

First column: compound identification.

Second column: temperature range of comparison.

Third column: average absolute percent deviation of the DIPPR values from our recommendations.

Fourth column: maximum percent deviation of the DIPPR values from our recommendations.

Fifth column: ratio of the value in the third column and the sum of the reported percent uncertainties in our recommendations and those in the DIPPR data base.

Sixth column: ratio of the value in the fourth column and the sum of the reported percent uncertainties in our recommendations and those in the DIPPR data base.

For most compounds the differences change sign over the temperature range where comparisons were performed. Our data are systematically higher for ethanol and n-nonane and lower for 1-butanol. The items in the last two columns are in most cases below 1 which indicates that the differences were usually smaller than the sum of expected errors of the two recommendations (error limits of the DIPPR data base are generally larger compared to ours). Important disagreement was observed only for 1-propanol where some systematic error can be expected in the DIPPR data base.

5. Tables and Figures

Table 1. Experimental heat capacities for methane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type capacity	Calorimeter type-reference
24EUC/KAR	96.3–108.7	7	3.00	not specified	C_{sat}	IP-24EUC/KAR
29CLU	95.4–105.3	6	0.70	not specified	C_p	IP-29CLU
30WIE/BRE	110.9–188.2	18	2.00	not specified	C_{sat}	IP-30WIE/HUB
61HES/WHI	114.5–187.5	9	nosp	99.96 melpt	C_{sat}	IP-53RIF/KER
63COL/GIL	93.4	1	nosp	99.995 chrom	C_p	AD-61FLU/LEA
65CUT/MOR	93.9–107.0	5	0.20	99.98 chrom	C_{sat}	AD-61FLU/LEA
74YOU	95.4–187.6	66	0.50	99.99 melpt	C_{sat}	AD-61GOO

Table 2. Correlated heat capacities for methane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_h/R	+/−
				Selected data				
29CLU	95.4–105.3	5	0.70	0.396	1.81–2	0.28	− 1.81–3	1
63COL/GIL	93.4	1	0.70#	0.721	3.22–2	0.50	− 3.22–2	− 1
65CUT/MOR	93.9–107.0	4	0.20	2.680	3.49–2	0.54	− 2.93–2	− 4
74YOU	95.4–184.2	61	0.50	1.802	8.12–2	0.90	1.42–2	11
				Rejected data				
24EUC/KAR	(2.82–1, 4.13, 2.69–1, 7)			30WIE/BRE		(1.52–1, 1.56, − 1.19–1, − 16)		
61HES/WHI	(3.80–1, 3.49, 2.59–1, 6)							

Table 3. Parameters of cubic spline polynomials for methane.

Heat cap. type	No. points total	No. points used	Statistics s_w	Statistics s/R	Statistics s_r %	Statistics s_b/R	Statistics +/−
C_p	112	71	2.344	1.21–1	1.13	1.15–2	7
C_{sat}	112	71	1.888	8.00–2	0.90	9.98–3	7

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
93.39–120.00	− 7.803 06	3.792 86 + 1	− 3.445 07 + 1	1.083 07 + 1	III
120.00–150.00	1.436 01 + 1	− 1.747 93 + 1	1.172 26 + 1	− 1.995 22	III
150.00–180.00	− 4.625 46 + 2	9.363 33 + 2	− 6.241 52 + 2	1.393 10 + 2	IV
180.00–184.22	− 1.684 08 + 5	2.808 45 + 5	− 1.561 29 + 5	2.893 65 + 4	V
93.39–120.00	2.201 71 − 1	1.550 58 + 1	− 1.362 04 + 1	4.391 83	III
120.00–150.00	6.347 68	1.870 47 − 1	− 8.547 78 − 1	8.458 26 − 1	III
150.00–180.00	− 2.793 61 + 2	5.716 05 + 2	− 3.818 00 + 2	8.550 04 + 1	IV
180.00–184.22	− 9.667 98 + 4	1.612 39 + 5	− 8.964 15 + 4	1.661 51 + 4	V

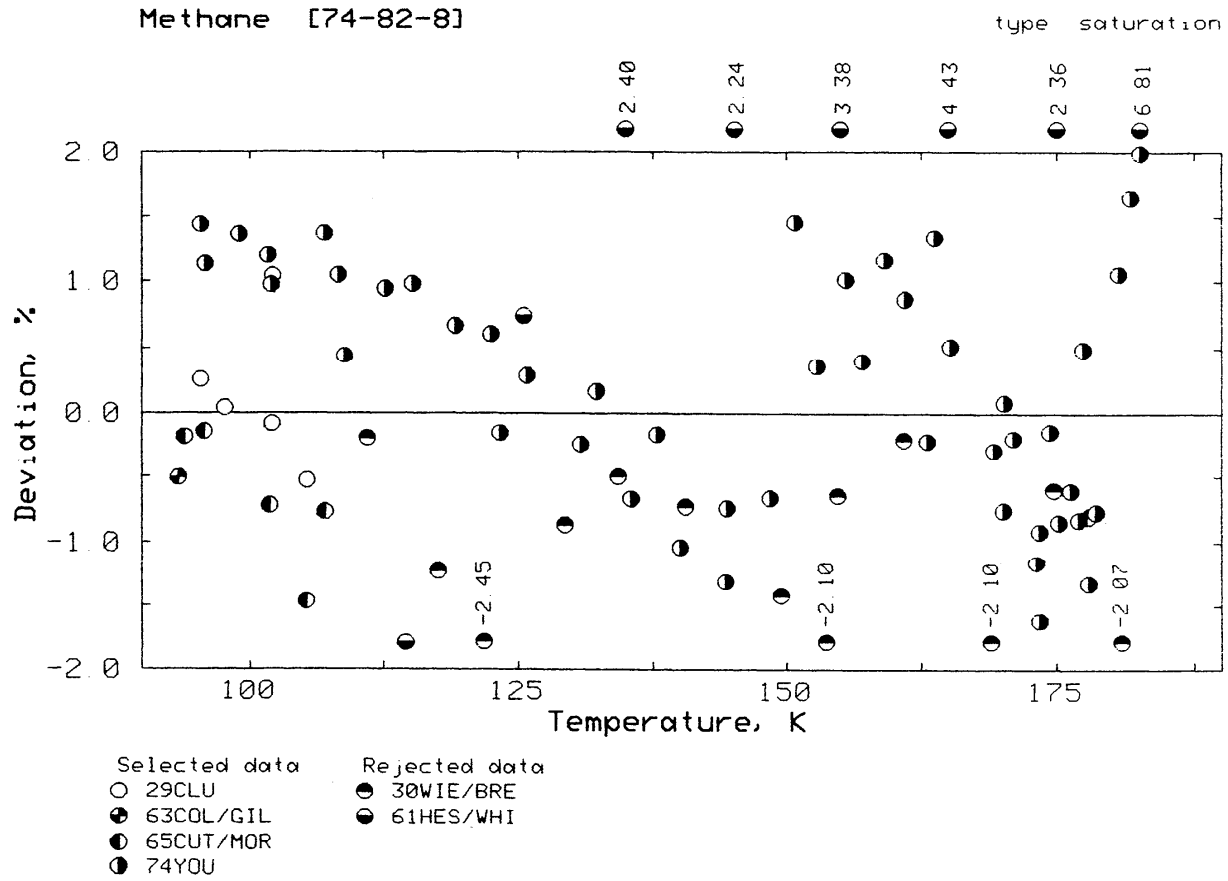

FIG. 1. Deviation plot for methane.

Table 4. Experimental heat capacities for ethane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
28EUC/HAU	100.0–270.0	18S	nosp	not specified	C_{sat}	IP–28EUC/HAU
30WIE/HUB *N*	96.8–138.2	15	1.00	99.0 estim	C_{sat}	IP–30WIE/HUB
37WIT/KEM	91.6–180.9	29	0.40	99.5 melpt	C_p	IP–28GIA/WIE
76ROD1	92.2	1	nosp	not specified	C_p	AD–61GOO
76ROD2	93.7–301.5	106	0.50	99.98 chrom	C_{sat}	AD–61GOO

30WIE/HUB error 0.5 and 1.0% below and above normal boiling temperature, respectively.

Table 5. Correlated heat capacities for ethane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
30WIE/HUB	96.8–138.2	15	1.00	0.400	3.32–2	0.40	4.30–3	1
37WIT/KEM	91.6–180.9	29	0.40	0.901	3.06–2	0.36	4.40–3	11
76ROD1	92.2	1	0.30#	1.365	3.37–2	0.41	3.37–2	1
76ROD2	93.7–300.5	105	0.50	1.069	7.25–2	0.53	−1.92–3	−19
	Rejected data							
28EUC/HAU	(1.70, 15.62, 1.64, 18)							

Table 6. Parameters of cubic spline polynomials for ethane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	169	150	1.386	1.05–1	0.69	1.02–3	0
C_{sat}	169	150	1.017	6.46–2	0.50	1.59–4	−6

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
91.59–150.00	5.154 96	7.373 97	−5.930 51	1.645 14	III
150.00–220.00	1.161 24 + 1	−5.540 85	2.679 36	−2.681 63 − 1	III
220.00–285.00	−1.459 56 + 2	2.093 26 + 2	−9.498 73 + 1	1.452 98 + 1	IV
285.00–300.55	−6.632 14 + 4	6.986 77 + 4	−2.453 65 + 4	2.873 19 + 3	IV
91.59–150.00	5.785 44	5.827 71	−4.693 10	1.322 12	III
150.00–220.00	1.088 30 + 1	−4.367 37	2.103 63	−1.882 62 − 1	III
220.00–285.00	−9.310 14 + 1	1.374 30 + 2	−6.234 95 + 1	9.577 37	IV
285.00–300.55	−3.811 64 + 4	4.016 20 + 4	−1.410 60 + 4	1.652 11 + 3	IV

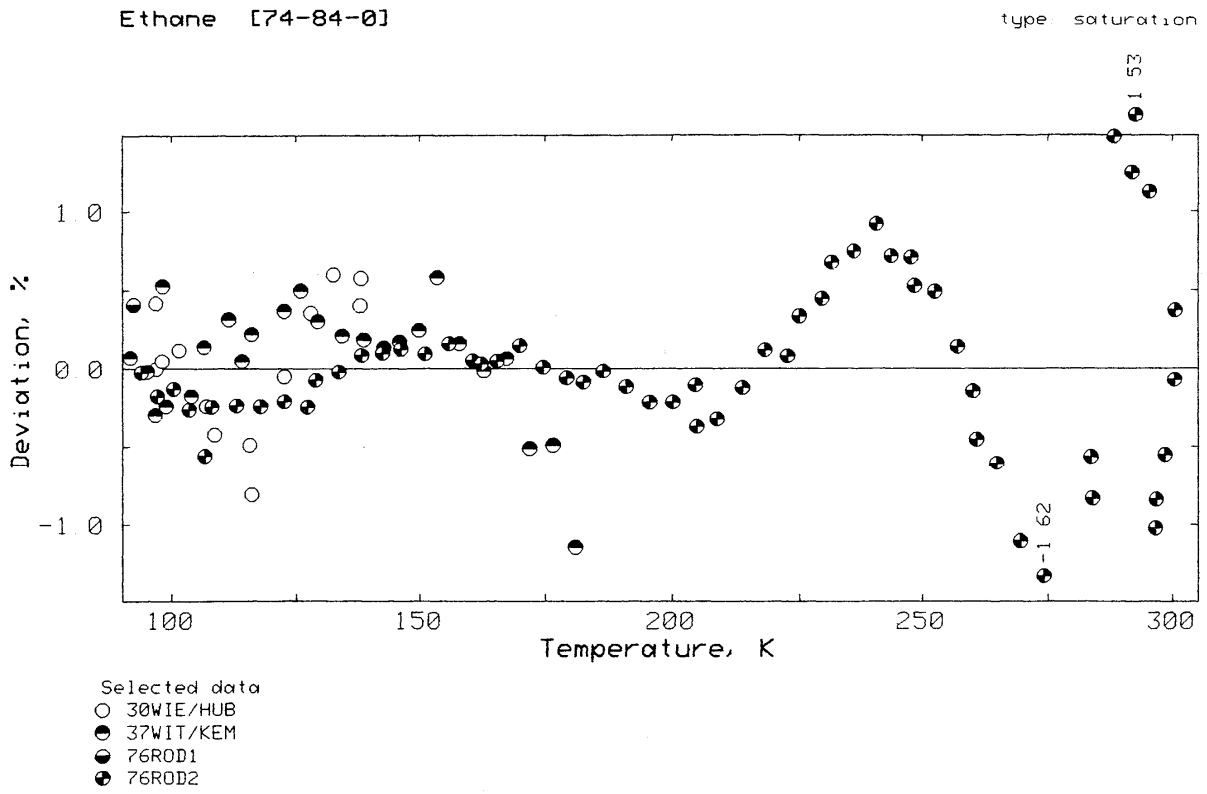

FIG. 2. Deviation plot for ethane.

Table 7. Experimental heat capacities for propane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
26DAN/JEN	241.8–291.6	12	2.00	not specified	C_{sat}	IP–26DAN/JEN
38KEM/EGA	89.7–229.8	22	nosp	99.9 melpt	C_p	IP–28GIA/WIE
65CUT/MOR	91.1–104.8	7	0.20	99.99 chrom	C_{sat}	AD–61FLU/LEA
78GOO	81.1–288.8	78	2.00	99.99 melpt	C_{sat}	AD–61GOO

Table 8. Correlated heat capacities for propane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
38KEM/EGA	89.7–229.8	22	0.50#	0.517	2.80–2	0.26	7.99–4	0
65CUT/MOR	91.1–104.8	7	0.20	1.679	3.40–2	0.34	−1.75–2	−3
78GOO	81.1–288.8	78	0.50#	0.499	2.55–2	0.25	9.88–3	36
				Rejected data				
26DAN/JEN	(4.87 − 1, 4.04, − 3.45 − 1, − 9)							

Table 9. Parameters of cubic spline polynomials for propane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	119	107	0.668	2.75–2	0.27	6.22–3	33
C_{sat}	119	107	0.668	2.75–2	0.27	6.22–3	33

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
81.05–115.00	1.067 21 + 1	− 2.478 79	2.765 88	− 7.798 94 − 1	II
115.00–200.00	8.919 13	2.094 04	− 1.210 50	3.726 79 − 1	III
200.00–288.81	8.452 15	2.794 52	− 1.560 74	4.310 52 − 1	III
81.05–115.00	1.061 82 + 1	− 2.320 26	2.612 44	− 7.311 05 − 1	II
115.00–200.00	8.969 72	1.979 99	− 1.126 89	3.527 59 − 1	III
200.00–288.81	9.778 91	7.662 09 − 1	− 5.200 00 − 1	2.516 10 − 1	III

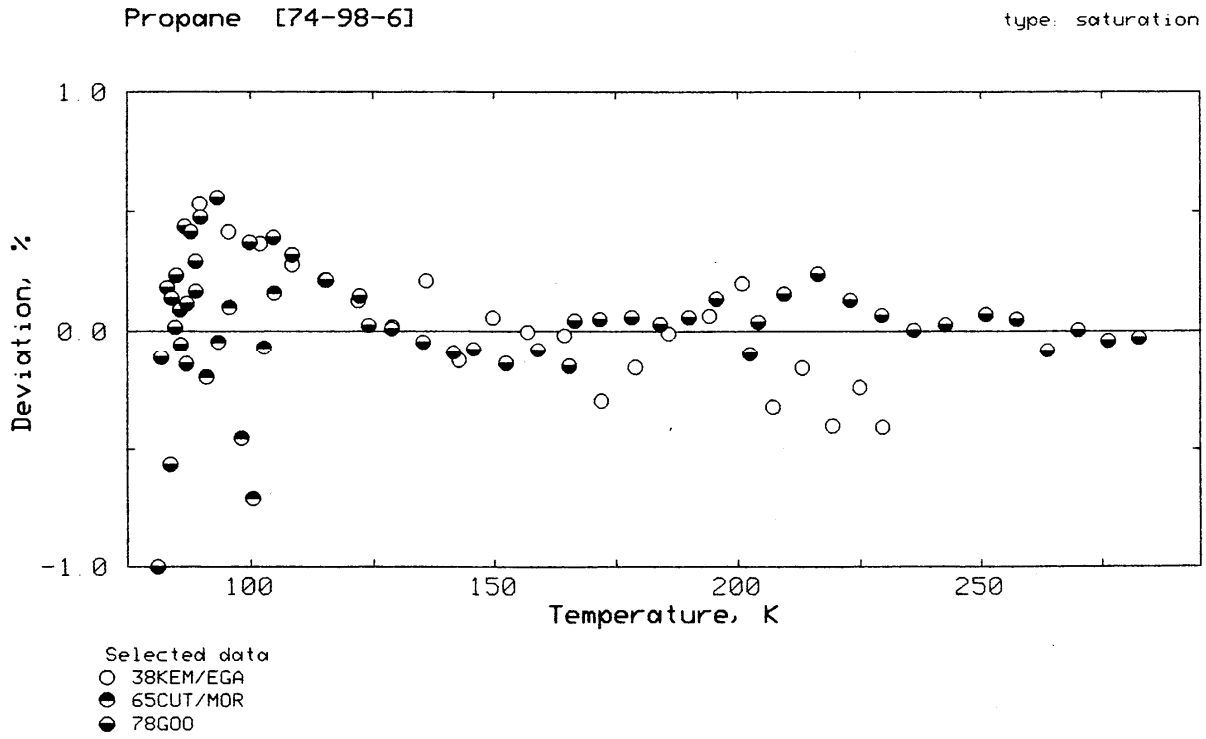

FIG. 3. Deviation plot for propane.

Table 10. Experimental heat capacities for butane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
26DAN/JEN	256.9–294.4	10	2.00	not specified	C_{sat}	IP–26DAN/JEN
31HUF/PAR	139.7–261.8	8	1.00	not specified	C_p	IP–31PAR
35SAG/LAC *N*	294.5–365.0	18	nosp	99.21 anal	C_{sat}	AD–35SAG/LAC
40AST/MES	139.9–268.1	21	nosp	99.999 melpt	C_p	IP–36AST/MES

35SAG/LAC data plotted on a graph.

Table 11. Correlated heat capacities for butane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
			Selected data					
35SAG/LAC	295.4–365.0	18	1.50#	0.827	2.22–1	1.24	−4.25–2	−4
40AST/MES	139.9–268.1	21	0.30#	1.079	4.82–2	0.32	1.96–3	−1
			Rejected data					
26DAN/JEN	(3.70 − 1, 2.21, 1.57 − 1, 4)			31HUF/PAR		(1.03–1, 0.72, −9.27–2, −7)		

Table 12. Parameters of cubic spline polynomials for butane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	57	39	1.060	1.70–1	0.95	−1.84–2	−5
C_{sat}	57	39	1.056	1.68–1	0.95	−1.86–2	−5

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
139.88–212.47	5.679 77	1.217 59 + 1	−6.315 07	1.201 30	III
212.47–305.37	1.600 48 + 1	−2.402 70	5.464 03 − 1	1.248 37 − 1	IV
305.37–364.98	−1.140 28 + 2	1.253 43 + 2	−4.128 68 + 1	4.691 23	V
139.88–212.47	5.808 34	1.195 73 + 1	−6.193 11	1.178 95	III
212.47–305.37	1.654 88 + 1	−3.207 83	9.444 48 − 1	5.917 46 − 2	IV
305.37–364.98	−8.518 45 + 1	9.673 65 + 1	−3.178 45 + 1	3.631 77	V

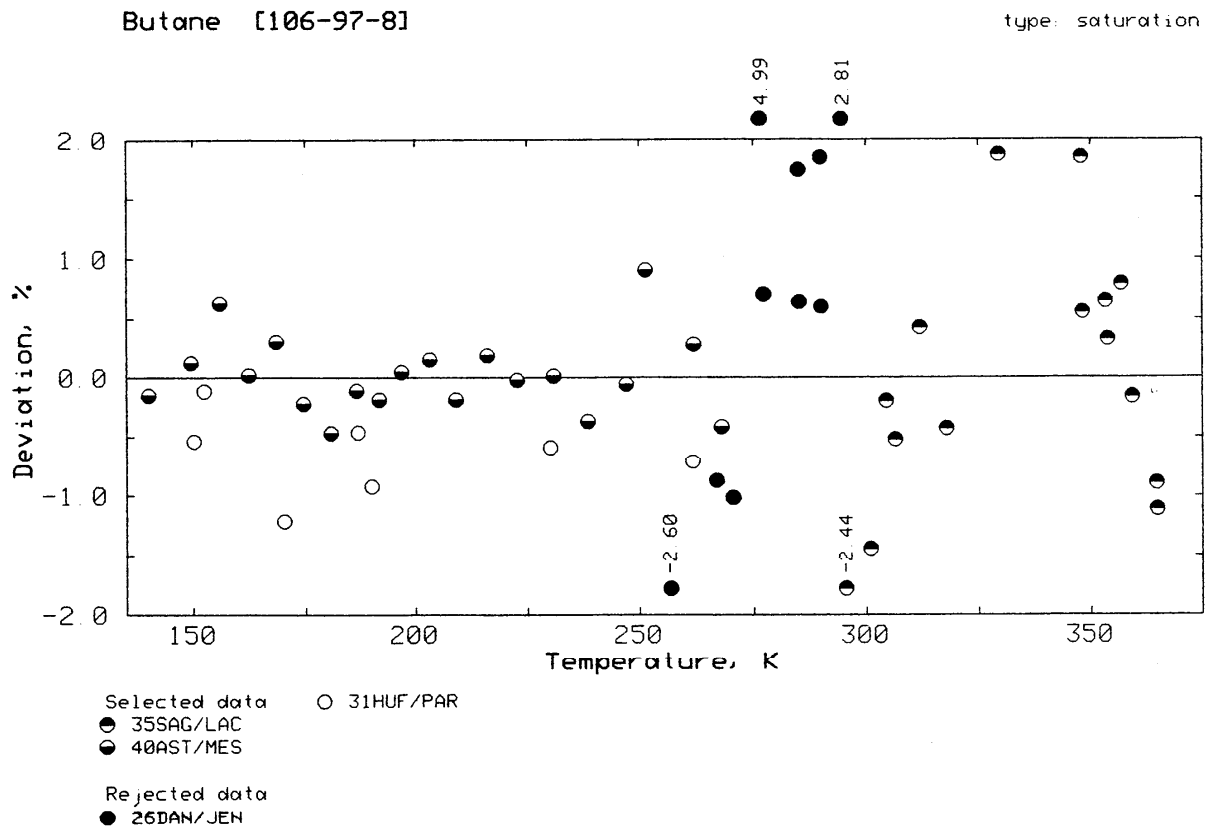

FIG. 4. Deviation plot for butane.

Table 13. Experimental heat capacities for pentane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
30PAR/HUF1	149.9–290.0	14	1.00	not specified	C_p	IP–25PAR
40MES/KEN	151.3–286.4	19	nosp	99.961 melpt	C_p	IP–36AST/MES
67MES/GUT	148.6–302.9	25	0.10	99.86 melpt	C_{sat}	AD–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	AD–75RAS/GRI
85CZA	299.0	1	nosp	not specified	C_p	IP–79CZA
88MEL/VER	153.1–433.1	10	2.50	not specified	C_{sat}	not specified

71AMI/ALI calculated from C_v measured at saturated line.
75GRI/RAS all values (except the first one) at pressure above p_{sat}.

Table 14. Correlated heat capacities for pentane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
67MES/GUT	148.6–302.9	25	0.10	0.202	3.75–3	0.02	2.16–4	3
75GRI/RAS	299.9–383.6	9	1.00	0.495	1.08–1	0.49	− 6.24–2	− 5
88MEL/VER	153.1–393.1	9	2.50	0.197	1.07–1	0.49	2.55–2	1
				Rejected data				
30PAR/HUF1	(1.11 − 1, 0.60, − 9.00 − 2, − 12)			40MES/KEN		(1.28 − 1, 0.65, 2.23 − 2, − 5)		
71AMI/ALI	(3.94 − 1, 1.80, 3.38 − 1, 9)			85CZA		(2.86 − 1, 1.44, − 2.86 − 2, − 1)		

Table 15. Parameters of cubic spline polynomials for pentane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	97	43	0.338	7.90–2	0.36	− 8.23–3	1
C_{sat}	97	43	0.311	7.50–2	0.34	− 7.60–3	− 1

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
148.60–210.00	2.064 89 + 1	− 4.670 97	1.478 02	1.788 95 − 2	II
210.00–290.00	2.351 67 + 1	− 8.767 90	3.428 94	− 2.917 80 − 1	II
290.00 393.15	1.333 17 + 1	1.768 28	2.042 28 − 1	1.258 25 − 1	IV
148.60–210.00	2.048 89 + 1	− 4.402 58	1.329 47	4.500 19 − 2	II
210.00–290.00	2.410 35 + 1	− 9.566 35	3.788 41	− 3.453 06 − 1	II
290.00–393.15	1.549 05 + 1	− 6.563 08 − 1	7.159 84 − 1	7.846 18 − 3	IV

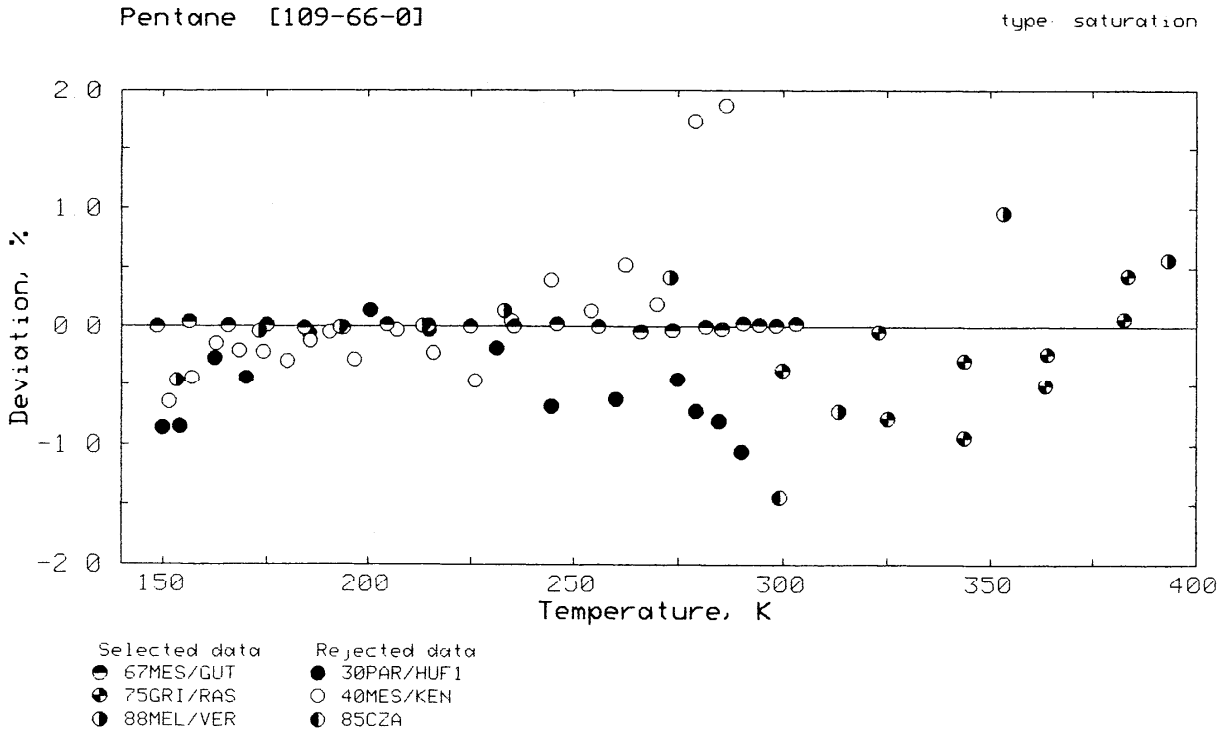

FIG. 5. Deviation plot for pentane.

Table 16. Experimental heat capacities for hexane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
30PAR/HUF2	183.5–295.1	8	nosp	not specified	C_p	IP–25PAR
31HUF/PAR	188.8–293.5	5	1.00	not specified	C_p	IP–25PAR
37STU	180.0–320.0	15S	nosp	not specified	C_p	CC–37STU
39PHI	300.6	1	nosp	not specified	C_p	IP–49WEI
46 DOU/HUF *N*	180.4–301.0	24	0.10	99.992 melpt	C_p	AD–43RUE/HUF
51CON/SAG	299.8–366.5	13S	0.70	not specified	C_p	AD–39SAG/EVA
69WIL/ROT	293.1	1	0.40	not specified	C_p	AD–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	IP–70REC
74DIA/REN	298.2–324.7	14	0.30	not specified	C_p	AD–74DIA/REN
75GRI/RAS *N*	304.5–463.1	9	1.00	not specified	C_p	AD–75RAS/GRI
76KAR/GRO	298.2	1	nosp	not specified	C_p	FL–71PIC/LED
80KAL/JED	180.6–301.4	33	0.20	99.95 chrom	C_p	AD–80KAL/JED
81GRO/ING	298.1	1	nosp	99.5 chrom	C_p	FL–71PIC/LED
82WIL/ING	298.1	1	nosp	99.5 estim	C_p	FL–71PIC/LED
84BEN/DAR	298.1	1	nosp	99.98 melpt	C_p	FL–71PIC/LED
84BRA/PIN	298.1	1	nosp	99.0 melpt	C_p	FL–71PIC/LED
85COS/PAT1	298.2	1	nosp	99.0 anal	C_p	FL–71PIC/LED
85COS/PAT6	298.1–313.1	2	nosp	99.0 estim	C_p	FL–71PIC/LED
85CZA	299.9	1	nosp	not specified	C_p	IP–79CZA
86BEN/DAR1	298.1	1	nosp	99.88 anal	C_p	FL–71PIC/LED
86NAZ/BAS2	308.4–333.1	2	2.00	99.8 estim	C_p	RP–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	FL–71PIC/LED

46DOU/HUF smoothed data in 67MES/GUT.
71AMI/ALI calculated from C_v measured on saturation line.
75GRI/RAS all values (except the first one) at pressure above p_{sat}.

Table 17. Correlated heat capacities for hexane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
			Selected data					
31HUF/PAR	188.8–293.5	5	1.00	0.219	4.95–2	0.22	−3.28–2	−3
46DOU/HUF	180.4–301.0	24	0.10	0.864	1.83–2	0.09	−2.25–3	−2
51CON/SAG	299.8–366.5	13	0.70	0.329	5.93–2	0.23	4.90–2	9
69WIL/ROT	293.1	1	0.40	0.984	9.13–2	0.39	−9.13–2	−1
75GRI/RAS	304.5–463.1	9	1.00	0.491	1.40–1	0.49	−2.50–2	−1
76KAR/GRO	298.2	1	0.50#	0.504	5.94–2	0.25	5.94–2	1
80KAL/JED	180.6–301.4	33	0.20	1.230	5.23–2	0.25	6.35–3	−1
81GRO/ING	298.1	1	0.50#	0.053	6.20–3	0.03	6.20–3	1
82WIL/ING	298.1	1	0.50#	0.295	3.47–2	0.15	−3.47–2	−1
84BEN/DAR	298.1	1	0.50#	0.185	2.18–2	0.09	2.18–2	1
84BRA/PIN	298.1	1	0.50#	0.295	3.47–2	0.15	−3.47–2	−1
86BEN/DAR1	298.1	1	0.50#	0.226	2.67–2	0.11	2.67–2	1
88MEL/VER	183.1–41.1	10	2.50	0.129	7.69–2	0.32	−2.93–2	0
88SAI/TAN	298.1	1	0.50#	0.022	2.59–3	0.01	2.59–3	1

Rejected data

30PAR/HUF2	(2.33 − 1, 1.05, −2.14 − 1, −8)	37STU	(1.25, 5.22, 6.35 − 1, 4)
39PHI	(1.26, 5.61, −1.26, −1)	71AMI/ALI	(5.14 − 1, 1.80, −3.00 − 1, −6)
71REC/SAD	(2.99 − 1, 1.28, −2.99 − 1, −1)	74DIA/REN	(6.27 − 1, 2.48, 5.66 − 1, 14)
85COS/PAT1	(2.43 − 1, 1.02, 2.43 − 1, 1)	85COS/PAT6	(2.83 − 1, 1.15, 1.57 − 1, 0)
85CZA	(1.75 − 1, 0.75, −1.75 − 1, −1)	86NAZ/BAS2	(5.10 − 1, 2.02, 5.06 − 1, 2)

Table 18. Parameters of cubic spline polynomials for hexane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	167	102	0.884	7.39–2	0.29	1.06–3	2
C_{sat}	167	102	0.874	6.51–2	0.26	6.56–4	4

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
180.42–250.00	4.133 02 + 1	− 2.746 31 + 1	1.132 79 + 1	− 1.388 61	II
250.00–330.00	1.533 21 + 1	3.734 46	− 1.151 11	2.752 63 − 1	III
330.00–463.11	5.250 15 + 1	3.005 58 + 1	9.088 36	7.590 28 − 1	IV
180.42–250.00	4.132 70 + 1	− 2.745 57 + 1	1.132 30 + 1	− 1.387 61	II
250.00–330.00	1.574 09 + 1	3.247 64	− 9.583 38 − 1	2.498 96 − 1	III
330.00–463.11	6.499 16 + 1	− 4.152 58 + 1	1.260 94 + 1	− 1.120 58	IV

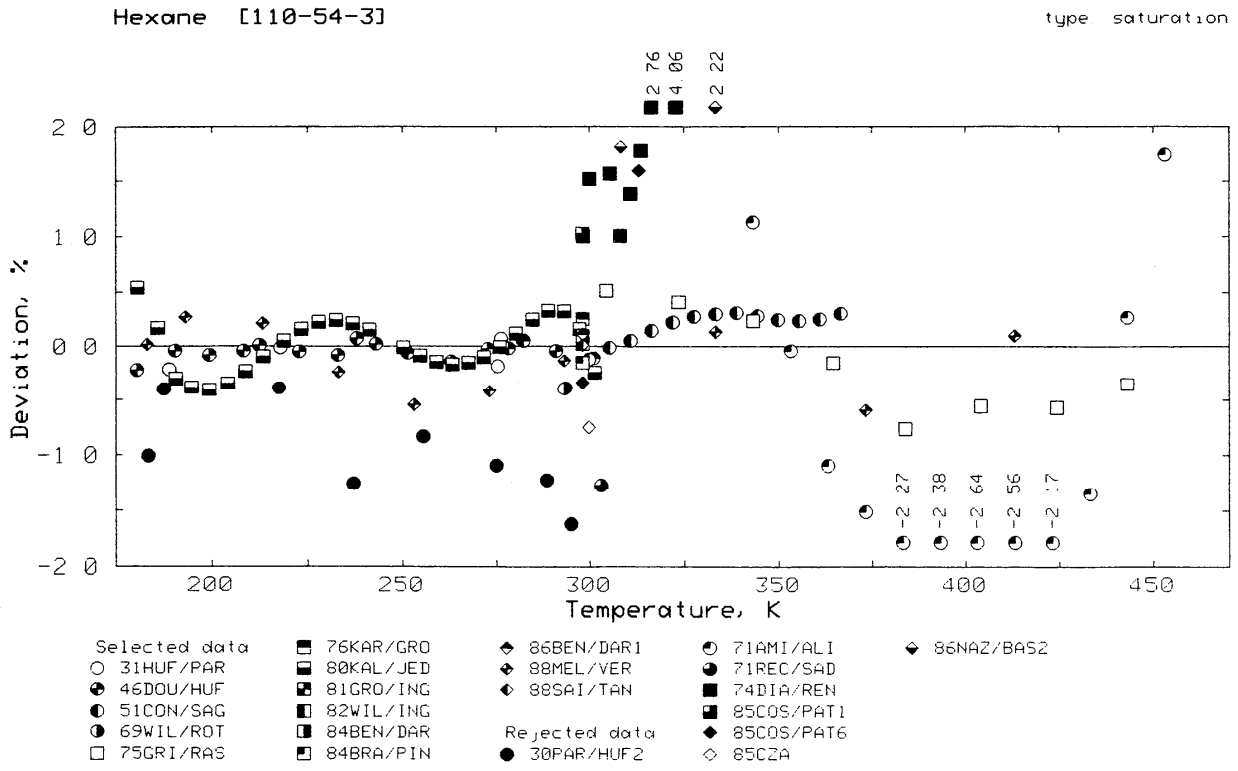

FIG. 6. Deviation plot for hexane.

Table 19. Experimental heat capacities for heptane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
24WIL/DAN	309.0–380.0	Eq.	nosp	not specified	C_p	AD–24WIL/DAN
30PAR/HUF2	188.0–299.2	14	nosp	not specified	C_p	IP–25PAR
37VOL	298.1	1	nosp	not specified	C_p	IP–37VOL
39BYK	298.1–298.1	2	nosp	not specified	C_p	IP–39BYK
39PHI	300.8	1	nosp	not specified	C_p	IP–49WEI
40PIT	194.6–317.6	6	0.50	99.85 melpt	C_p	IP–28LAT/GRE
47OSB/GIN *N*	280.6–358.1	9S	0.10	99.96 estim	C_{sat}	AD–470SB/GIN
47OSB/GIN *N*	285.6–305.6	5S	0.10	99.96 estim	C_{sat}	AD–470SB/GIN
54DOU/FUR *N*	185.0–520.0	47S	0.10	99.999 melpt	C_{sat}	AD–54SCO/MEY
58SWI/ZIE *N*	332.6	1	nosp	not specified	C_{avg}	DR–58SWI/ZIE
61HUF/GRO *N*	182.6–370.0	22S	0.10	not specified	C_{sat}	AD–43RUE/HUF
61MCC/MES *N*	188.5–307.8	20	nosp	99.97 melpt	C_{sat}	AD–43RUE/HUF
61MCC/MES *N*	183.0–320.8	25	nosp	99.996 melpt	C_{sat}	AD–43RUE/HUF
61MCC/MES *N*	188.9–320.4	23	nosp	99.996 melpt	C_{sat}	AD–43RUE/HUF
61MCC/MES *N*	192.9–340.8	17	nosp	99.996 melpt	C_{sat}	AD–43RUE/HUF
61MCC/MES *N*	190.9–367.0	19	nosp	99.94 melpt	C_{sat}	AD–43RUE/HUF
66KLE	293.1–343.1	11S	0.10	not specified	C_p	AD–66KLE
70AKII	293.1	1	nosp	not specified	C_p	CC–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	AD–72VAN
75GRI/RAS *N*	303.5–342.9	3	nosp	not specified	C_p	AD–75RAS/GRI
75HOL/ZIE	182.0–312.0	Eq.	0.20	99.73 anal	C_p	AD–45SCO/MEY
75SAN *N*	413.1–513.2	8S	1.00	not specified	C_p	FL–75SAN
77MEI/BLO	187.0–354.6	35	nosp	not specified	C_{sat}	AD–72VAN
79BRO/ZIE	183.0–302.0	Eq.	nosp	99.7 melpt	C_p	AD–45SCO/MEY
79SCH/OFF	190.0–285.0	20S	nosp	99.88 melpt	C_{sat}	AD–79SCH/OFF
80KAL/JED	185.0–301.0	96	0.20	99.95 chrom	C_p	AD–80KAL/JED
83TAN/ZHO	214.2–365.2	40	0.20	99.99 chrom	C_{sat}	AD–83TAN/ZHO
84GRI/AND	293.0–323.6	14	0.50	not specified	C_p	AD–67RAS/GAN
84GUS/MIR	303.1–363.1	4S	1.60	not specified	C_p	DC–84GUS/MIR
85CZA	299.3	1	nosp	not specified	C_p	IP–79CZA
87VAN/VAN	184.2–345.7	37	0.20	99.75 melpt	C_p	AD–87VAN/VAN
87WIL/ING	298.1	1	nosp	99.5 anal	C_p	FL–71PIC/LED
88MEL/VER	193.1–523.2	11	2.50	not specified	C_{sat}	not specified

47OSB/GIN calorimeter with vessel of large volume.
47OSB/GIN calorimeter with vessel of small volume.
54DOU/FUR the same data in 53GIN/FUR; AD calorimeter used to 370 K and DI calorimeter by 50GIN/DOU used from 273 to 523 K.
58SWI/ZIE average value in temperature range 294–369 K.
61HUF/GRO the 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); the results are less accurate near and above room temperature.
61MCC/MES measured in 1954.
71AMI/ALI calculated from C_v measured on saturation line.
75GRI/RAS sample grade: pure.
75SAN the same data in 76SAN/MEL; C_p at p_{sat} obtained by extrapolation from high pressure measurements.

Table 20. Correlated heat capacities for heptane.

Reference	Temp. range K	No. points used	$\sigma_r C^1$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
47OSB/GIN	200.6–358.1	9	0.10	0.504	1.37–2	0.05	7.61–3	3
47OSB/GIN	285.6–305.6	5	0.10	0.166	4.45–3	0.02	1.89–3	− 1
54DOU/FUR	185.0–520.0	47	0.10	0.564	2.01–2	0.06	5.11–6	7
61HUF/GRO	182.6–370.0	22	0.10	0.750	1.94–2	0.07	1.46–2	18
66KLE	293.1–343.1	11	0.10	0.431	1.18–2	0.04	− 7.86–3	− 5
79SCH/OFF	190.0–285.0	20	0.10#	0.589	1.45–2	0.06	− 7.52–3	− 10
80KAL/JED	185.0–301.0	95	0.20	0.280	1.39–2	0.06	− 6.76–3	− 31
87WIL/ING	298.1	1	0.50#	0.003	4.66–4	0.00	4.66–4	1

Rejected data

24WIL/DAN	(5.33–1, 1.96, − 2.86 − 1, − 1)	30PAR/HUF2	(1.90 − 1, 0.73, − 1.56 − 1, − 12)
37VOL	(2.40 − 1, 0.90, − 2.40 − 1, − 1)	39BYK	(1.56, 6.14, − 1.56, − 2)
39PHI	(1.78, 7.01, − 1.78, − 1)	40PIT	(1.19 − 1, 0.46, 8.56 − 2, 4)
58SWI/ZIE	(1.06, 3.56, 1.06, 1)	70AKH	(8.04 − 2, 0.30, − 8.04 − 2, − 1)
71AMI/ALI	(8.06 − 1, 2.31, − 5.76 − 1, − 11)	72VAN	(7.97 − 2, 0.33, 5.19 − 2, 8)
75GRI/RAS	(1.07 − 1, 0.38, 2.62 − 4, 1)	75HOL/ZIE	(3.53 − 2, 0.13, − 3.00 − 2, − 19)
75SAN	(8.36 − 1, 2.29, − 6.44 − 1, − 2)	77MEI/BLO	(6.15 − 2, 0.22, − 2.03 − 2, − 7)
79DRO/ZIE	(7.19 − 1, 2.89, − 6.92 − 1, − 20)	83TAN/ZHO	(3.97 − 2, 0.15, − 2.77 − 2, − 26)
84GRI/AND	(4.11 − 1, 1.48, 4.08 − 1, 14)	84GUS/MIR	(4.17 − 1, 1.45, − 3.93 − 1, − 4)
85CZA	(4.13 − 2, 0.15, 4.13 − 2, 1)	87VAN/VAN	(5.10 − 2, 0.20, − 3.61 − 2, − 21)
88MEL/VER	(1.23 − 1, 0.35, 7.66 − 2, 8)		

Table 21. Parameters of cubic spline polynomials for heptane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	451	210	0.538	1.89–2	0.06	− 2.18–3	− 28
C_{sat}	451	210	0.477	1.62–2	0.06	− 2.28–3	− 18

Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
		Parameters			
182.55–260.00	6.057 96 + 1	− 4.450 53 + 1	1.727 71 + 1	− 2.058 23	I
260.00–400.00	2.658 39 + 1	− 5.279 42	2.190 23	− 1.240 16 − 1	I
400.00–490.00	− 1.060 24 + 2	9.417 68 + 1	− 2.267 38 + 1	1.947 99	II
490.00–520.00	− 2.004 21 + 4	1.229 99 + 4	− 2.513 64 + 3	1.714 02 + 2	II
182.55–260.00	6.078 64 + 1	− 4.476 54 + 1	1.738 43 + 1	− 2.072 69	I
260.00–400.00	2.700 36 + 1	− 5.785 20	2.391 91	− 1.505 89 − 1	I
400.00–490.00	− 4.412 72 + 1	4.756 29 + 1	− 1.094 51 + 1	9.608 29 − 1	II
490.00–520.00	− 1.427 69 + 4	8.761 52 + 3	− 1.789 30 + 3	1.219 38 + 2	II

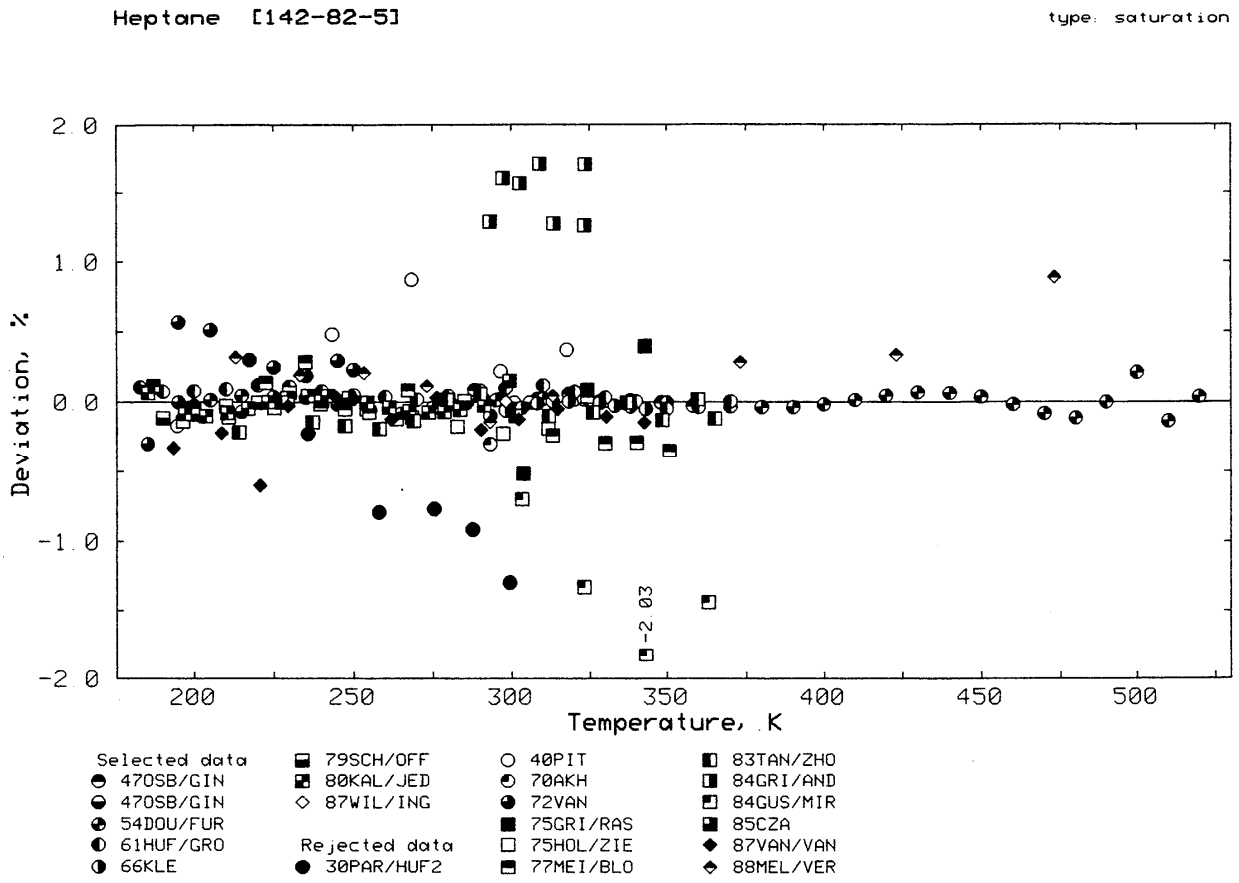

FIG. 7. Deviation plot for heptane.

Table 22. Experimental heat capacities for octane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
30PAR/HUF2	223.0–293.7	8	nosp	not specified	C_p	IP–25PAR
31HUF/PAR	227.0–298.3	5	nosp	not specified	C_p	IP–25PAR
47OSB/GIN	285.6–305.6	5S	0.10	99.96 estim	C_{sat}	AD–47OSB/GIN
49TSC/WET	298.1	1	nosp	not specified	C_p	IP–49TSC/RIC
51CON/SAG	299.8–366.5	13S	nosp	not specified	C_p	AD–39SAG/EVA
54FIN/GRO *N*	222.6–297.6	18	0.20	99.94 melpt	C_{sat}	AD–43RUE/HUF
61ROU	283.1–312.2	15	nosp	99.83 anal	C_p	AD–61ROU
70AKH	293.1	1	nosp	not specified	C_p	CC–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	AD–75RAS/GRI
80SHA/LYU	216.4–300.0	12S	0.50	99.57 melpt	C_p	AD–80SHA/LYU
81GRO/ING	298.1	1	nosp	99.0 chrom	C_p	FL–71PIC/LED
84GRI/AND *N*	297.5–386.1	7	0.50	not specified	C_p	AD–67RAS/GAN
84ROU/GRO	298.1	1	0.30	99.0 estim	C_p	FL–71PIC/LED
85COS/PAT	298.2	1	nosp	99.0 anal	C_p	FL–71PIC/LED
85LAI/GRO	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
85LAI/ROD	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
86BEN/DAR	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67 MES/GUT.
71AMI/ALI calculated from C_v measured on saturation line.
75GRI/RAS sample grade: pure, last five values at pressure above p_{sat}.
84GRI/AND sample grade: pure.

Table 23. Correlated heat capacities for octane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
47OSB/GIN	285.6–305.6	5	0.30#	2.130	1.96–1	0.64	1.96–1	5
54FIN/GRO	222.6–297.6	18	0.10#	0.556	1.67–2	0.06	− 5.47–3	− 4
75GRI/RAS	304.0–462.1	9	1.00	0.436	1.52–1	0.44	− 3.35–2	− 3
81GRO/ING	298.1	1	0.50#	0.380	5.81–2	0.19	− 5.81–2	− 1
84ROU/GRO	298.1	1	0.30	0.700	6.41–2	0.21	− 6.41–2	− 1
85LAI/GRO	298.1	1	0.50#	0.194	2.97–2	0.10	2.97–2	1
86BEN/DAR1	298.1	1	0.50#	0.437	6.70–2	0.22	6.70–2	1
				Rejected data				
30PAR/HUF2	(4.60 − 1, 1.59, − 4.48 − 1, − 8)			31HUF/PAR	(3.46 − 1, 1.19, − 3.41 − 1, − 5)			
49TSC/WET	(1.95 − 1, 0.63, 1.95 − 1, 1)			51CON/SAG	(5.02 − 1, 1.54, − 4.71 − 1, − 13)			
61ROU	(3.08 − 1, 1.02, − 1.50 − 1, − 7)			70AKH	(2.74 − 1, 0.89, 2.74 − 1, 1)			
71AMI/ALI	(1.37, 3.65, − 1.34, − 6)			80SHA/LYU	(1.08 − 1, 0.36, − 3.55 − 2, 2)			
84GRI/AND	(2.75 − 1, 0.82, − 2.61 − 1, − 7)			85COS/PAT2	(1.33 − 1, 0.43, 1.33 − 1, 1)			
85LAI/ROD	(1.00 − 1, 0.33, − 1.00 − 1, − 1)							

Table 24. Parameters of cubic spline polynomials for octane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	122	36	0.997	1.16–1	0.36	1.55–2	− 2
C_{sat}	122	36	0.997	1.16–1	0.36	1.54–2	− 2

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
222.61–300.00	6.417 61 + 1	− 4.117 74 + 1	1.459 79 + 1	− 1.530 18	II
300.00–462.99	2.287 50 + 1	1.236 96 − 1	8.308 36 − 1	− 5.054 76 − 4	III
222.61–300.00	6.398 75 + 1	− 4.095 72 + 1	1.451 26 + 1	− 1.519 21	II
300.00–462.09	2.459 39 + 1	− 1.563 56	1.381 35	− 6.019 01 − 2	III

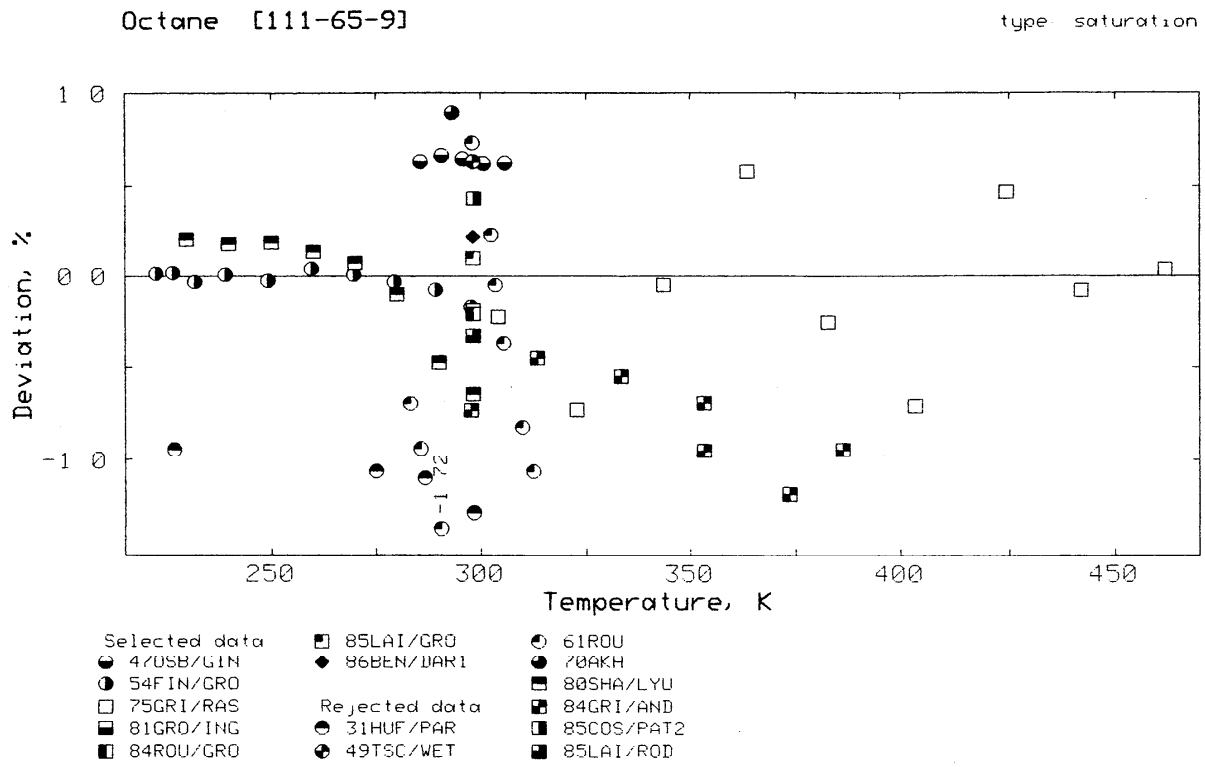

FIG. 8. Deviation plot for octane.

Table 25. Experimental heat capacities for nonane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
30PAR/HUF2	224.5–299.1	8	1.00	not specified	C_p	IP–25PAR
31HUF/PAR	228.3–297.9	8	1.00	not specified	C_p	IP–25PAR
47OSB/GIN	283.1–313.1	4S	0.10	99.96 estim	C_{sat}	AD–47OSB/GIN
54FIN/GRO *N*	225.0–313.9	22	0.20	99.88 melpt	C_{sat}	AD–43RUE/HUF
58SWI/ZIE *N*	348.8	1	nosp	not specified	C_{avg}	DR–58SWI/ZIE
70AKH	293.1	1	nosp	not specified	C_p	CC–59ABA/MUS
76MUS	307.8–417.9	10	2.50	not specified	C_p	AD–71MUS
79GRO/HAM	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
82WIL/ING	298.1	1	nosp	99.0 estim	C_p	FL–71PIC/LED
88AND/PAT	298.1	1	nosp	98.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT.
58SWI/ZIE average value in temperature range 295–402 K.

Table 26. Correlated heat capacities for nonane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
47OSB/GIN	283.1–313.1	4	0.10	1.453	4.98–2	0.15	−3.12–3	−2
54FIN/GRO	225.0–313.9	22	0.20	0.257	1.69–2	0.05	4.25–3	2
79GRO/HAM	298.1	1	0.30#	0.458	4.69–2	0.14	−4.69–2	−1
82WIL/ING	298.1	1	0.30#	0.810	8.30–2	0.24	−8.30–2	−1
88AND/PAT	298.1	1	0.30#	0.387	3.97–2	0.12	3.97–2	1
				Rejected data				
30PAR/HUF2	(4.23 − 1, 1.29, −4.21 − 1, −7)			31HUF/PAR		(3.03 − 1, 0.93, −2.96 − 1, −8)		
70AKH	(5.89 − 1, 1.70, 5.89 − 1, 1)			76MUS		(4.85 − 1, 1.42, −4.85 − 1, −1)		

Table 27. Parameters of regression polynomial for nonane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C	57	29	0.661	3.27–2	0.10	− 3.15–4	− 1

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
225.0–313.9	1.031 89 + 2	− 7.802 76 + 1	2.725 34 + 1	− 2.965 83	II

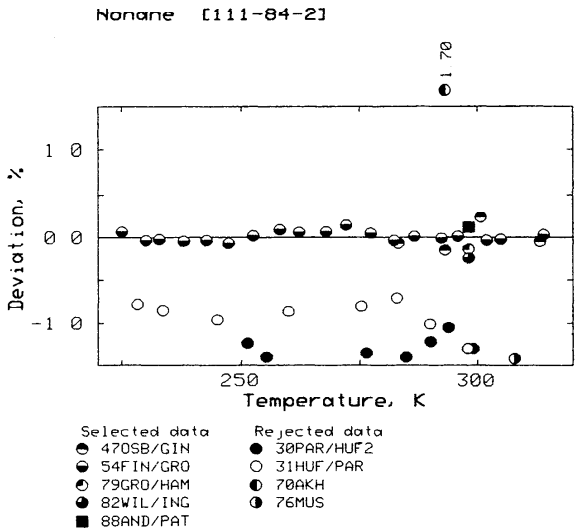

FIG. 9. Deviation plot for nonane.

TABLE 28. Experimental heat capacities for decane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
30PAR/HUF2	242.3–295.5	6	1.00	not specified	C_p	IP–25PAR
31HUF/PAR	251.2–297.7	6	1.00	not specified	C_p	IP–25PAR
47OSB/GIN	290.6–305.6	4S	0.10	99.96 estim	C_{sat}	AD–47OSB/GIN
52SCH/SAG	299.8–366.5	13S	1.00	99.7 estim	C_{sat}	AD–39SAG/EVA
54FIN/GRO *N*	247.0–318.6	17	0.20	99.91 melpt	C_{sat}	AD–43RUE/HUF
70AKH	293.1	1	nosp	not specified	C_p	CC–59ABA/MUS
75GRI/RAS *N*	303.3–462.4	9	1.00	not specified	C_p	AD–75RAS/GRI
79GRO/HAM	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
82WIL/ING	298.1	1	nosp	99.0 estim	C_p	FL–71PIC/LED
83SID/SVE	293.1	1	nosp	99.9 melpt	C_p	FL–71PIC/LED
84GRO/ING	298.1	1	nosp	99.0 melpt	C_p	FL–71PIC/LED
84ROU/GRO	298.1	1	nosp	98.0 estim	C_p	FL–71PIC/LED
85BAL/BRA	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
85COS/PAT3	298.2	1	nosp	99.0 anal	C_p	FL–71PIC/LED
85COS/PAT6	283.1–313.1	3	nosp	99.0 estim	C_p	FL–71PIC/LED
85LAI/ROD	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
85LAI/WIL	298.1	1	0.30	99.0 estim	C_p	FL–71PIC/LED
86GAT/WOO	298.1–368.1	4	nosp	99.0 anal	C_p	CT–83ROU/ROU
87WIL/ING	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
88COS/VAN	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
88KUZ/KHA	293.8–335.2	15	nosp	99.8 chrom	C_p	FL–75SAF/GER
88KUZ/KHA	310.1–421.9	16	nosp	not specified	C_p	AD–67RAS/GAN
88PIN/BRA	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT.
75GRI/RAS last two values at pressure above p_{sat}.

Table 29. Correlated heat capacities for decane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
54FIN/GRO	247.0–318.6	17	0.20	0.144	1.07–2	0.03	3.29–4	0
75GRI/RAS	303.3–462.4	9	1.00	0.703	2.96–1	0.70	− 6.81–2	− 1
84GRO/ING	298.1	1	0.30#	0.525	5.95–2	0.16	− 5.95–2	− 1
84ROU/GRO	298.1	1	0.30#	0.228	2.58–2	0.07	− 2.58–2	− 1
86GAT/WOO	298.1–368.1	4	0.30#	1.017	1.22–1	0.31	− 1.21–1	− 4
88KUZ/KHA	293.8–335.2	15	0.50#	0.417	8.03–2	0.21	7.37–2	15
88KUZ/KHA	310.1–421.9	16	0.60#	0.355	9.21–2	0.21	5.64–2	8

	Rejected data		
30PAR/HUF2	(6.59–1, 1.85, − 6.20 − 1, − 5)	31HUF/PAR	(3.10 − 1, 0.85, − 3.06 − 1, − 6)
47OSB/GIN	(3.28 − 1, 0.87, − 2.79 − 2, 0)	52SCH/SAG	(4.00 − 1, 1.03, − 3.56 − 1, − 11)
70AKH	(4.51 − 1, 1.22, − 4.51 − 1, − 1)	79GRO/HAM	(1.35 − 1, 0.36, − 1.35 − 1, − 1)
82WIL/ING	(2.29 − 1, 0.61, − 2.29 − 1, − 1)	83SID/SVE	(2.26 − 1, 0.61, − 2.26 − 1, − 1)
85BAL/BRA	(1.42 − 1, 0.38, − 1.42 − 1, − 1)	85COS/PAT3	(1.22 − 1, 0.32, 1.22 − 1, 1)
85COS/PAT6	(1.54 − 1, 0.40, 4.24 − 2, 1)	85LAI/ROD	(1.72 − 1, 0.46, − 1.72 − 1, − 1)
85LAI/WIL	(1.61 − 1, 0.43, − 1.61 − 1, − 1)	87WIL/ING	(1.81 − 1, 0.48, − 1.81 − 1, − 1)
88COS/VAN	(1.08 − 1, 0.28, 1.08 − 1, 1)	88PIN/BRA	(1.56 − 1, 0.41, − 1.56 − 1, − 1)

Table 30. Parameters of cubic spline polynomials for decane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C_p	107	63	0.489	1.37–1	0.33	1.32–2	16
C_{sat}	107	63	0.489	1.37–1	0.33	1.32–2	16

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
247.02–314.00	8.772 54 + 1	− 5.568 33 + 1	1.863 39 + 1	− 1.868 85	II
314.00–462.41	2.990 36 + 1	− 4.395 35 − 1	1.040 31	− 1.164 89 − 3	III
247.02–314.00	8.735 24 + 1	− 5.528 73 + 1	1.849 44 + 1	− 1.852 53	II
314.00–462.41	3.111 39 + 1	− 1.556 34	1.382 58	− 3.599 55 − 2	III

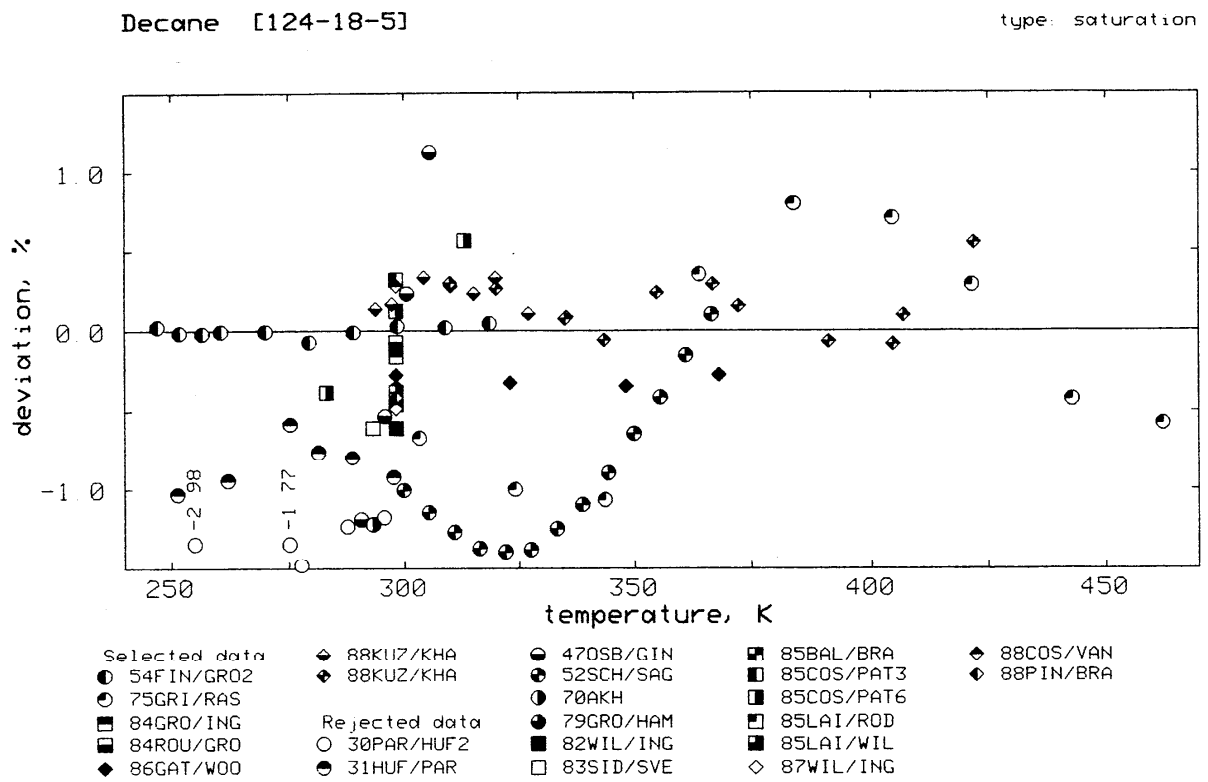

FIG. 10. Deviation plot for decane.

Table 31. Experimental heat capacities for undecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
31HUF/PAR	258.5–298.0	4	1.00	not specified	C_p	IP–25PAR
54FIN/GRO *N*	251.7–298.9	12	0.20	99.98 melpt	C_{sat}	AD–43RUE/HUF
70AKH	293.1	1	nosp	not specified	C_p	CC–59ABA/MUS
76MUS	307.8–458.6	14	2.50	not specified	C_p	AD–71MUS
84GRI/AND	292.3–433.4	8	0.80	not specified	C_p	AD–67RAS/GAN

54FIN/GRO smoothed data in 67MES/GUT.

Table 32. Correlated heat capacities for undecane.

Reference	Temp. range K	No. points used	$\sigma_r C'$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
54FIN/GRO	251.7–298.9	12	0.20	0.130	1.05–2	0.03	1.16–3	0
84GRI/AND	292.3–433.4	8	0.80	0.253	8.69–2	0.20	−2.75–2	0
				Rejected data				
31HUF/PAR	(1.95 − 1, 0.48, − 1.87 − 1, − 4)			70AKH		(4.82 − 1, 1.16, 4.82 − 1, 1)		
76MUS	(3.05, 6.87, − 2.94, − 11)							

Table 33. Parameters of cubic spline polynomials for undecane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C	39	20	0.220	6.51–2	0.15	− 1.02–2	0

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
251.74–290.00	2.012 87 + 2	− 1.700 58 + 2	5.827 00 + 1	− 6.442 76	II
290.00–433.42	6.293 13 + 1	− 2.693 17 + 1	8.916 09	− 7.699 06 − 1	IV

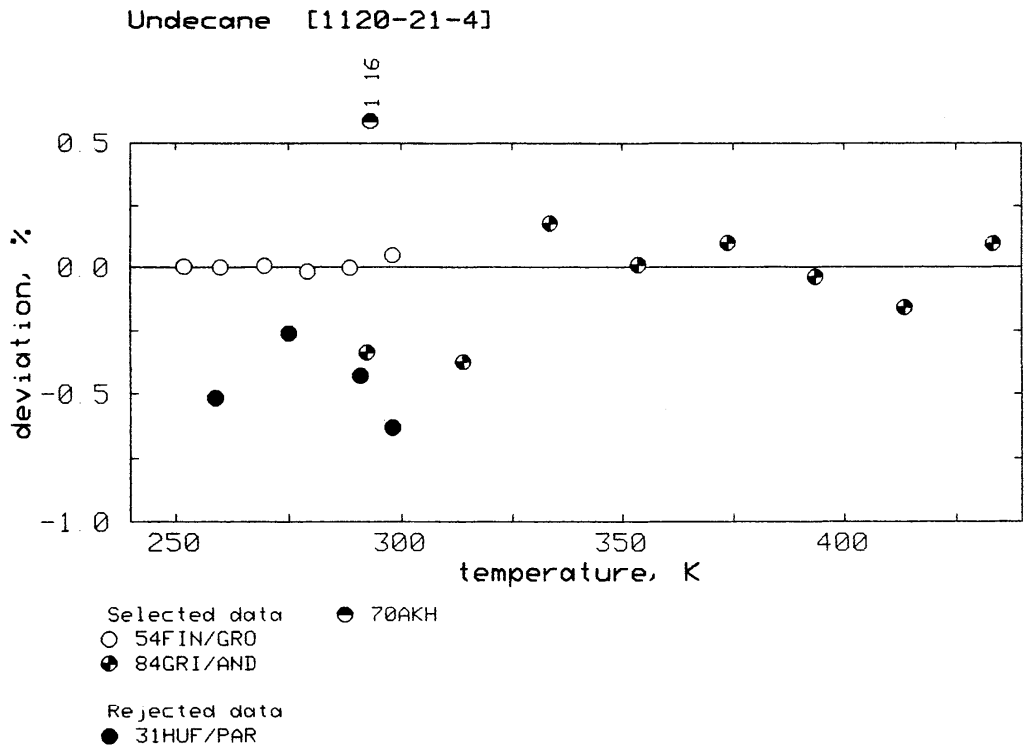

FIG. 11. Deviation plot for undecane.

Table 34. Experimental heat capacities for dodecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
31HUF/PAR	275.1–297.7	4	1.00	not specified	C_p	IP–25PAR
54FIN/GRO *N*	266.7–317.4	11	0.20	99.93 melpt	C_{sat}	AD–43RUE/HUF
71REC/SAD	303.1	1	0.30	not specified	C_p	IP–70REC
73KAL/WOY	303.1	1	0.20	99.5 chrom	C_p	IP–70REC
81GRO/ING	298.1	1	nosp	99.0 chrom	C_p	FL–71PIC/LED
84GRO/BEN	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
84KUM/BEN	298.1	1	nosp	98.0 estim	C_p	FL–71PIC/LED
85COS/PAT4	298.2	1	nosp	99.0 anal	C_p	FL–71PIC/LED
85COS/PAT6	283.1–313.1	3	nosp	99.0 estim	C_p	FL–71PIC/LED
85LAI/ROD	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
86BEN/DAR2	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
86WIL/LAI	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
88AND/PAT	298.1	1	nosp	98.0 anal	C_p	FL–71PIC/LED
88COS/VAN	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT.

Table 35. Correlated heat capacities for dodecane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
54FIN/GRO	266.7–317.4	11	0.20	0.264	2.36–2	0.05	1.03–3	2
84GRO/BEN	298.1	1	0.50#	0.308	6.94–2	0.15	− 6.94–2	− 1
84KUM/BEN	298.1	1	0.50#	0.286	6.46–2	0.14	− 6.46–2	− 1
85COS/PAT4	298.2	1	0.50#	0.074	1.66–2	0.04	1.66–2	1
86BEN/DAR2	298.1	1	0.50#	0.249	5.62–2	0.12	− 5.62–2	− 1
88AND/PAT	298.1	1	0.50#	0.331	7.49–2	0.17	7.49–2	1
88COS/VAN	298.1	1	0.50#	0.134	3.04–2	0.07	3.04–2	1
				Rejected data				
31HUF/PAR	(3.91 − 1, 0.88, − 3.83 − 1, − 4)			71REC/SAD		(4.26 − 1, 0.94, − 4.26 − 1, − 1)		
73KAL/WOY	(9.17 − 1, 2.06, − 9.17 − 1, − 1)			81GRO/ING		(1.22 − 1, 0.27, − 1.22 − 1, − 1)		
84ROU/GRO	(1.09 − 1, 0.24, − 1.09 − 1, − 1)			85COS/PAT6		(2.27 − 1, 0.50, 7.49 − 2, 1)		
85LAI/ROD	(3.05 − 1, 0.68, − 3.05 − 1, − 1)			86WIL/LAI		(3.05 − 1, 0.68, − 3.05 − 1, − 1)		

Table 36. Parameters of regression polynomial for dodecane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C	30	17	0.285	4.23–2	0.09	− 3.35–3	2

Temp. range K	Parameters A_0	A_1	A_2	Level of accuracy
266.7–317.4	6.082 57 + 1	− 1.631 85 + 1	3.715 84	II

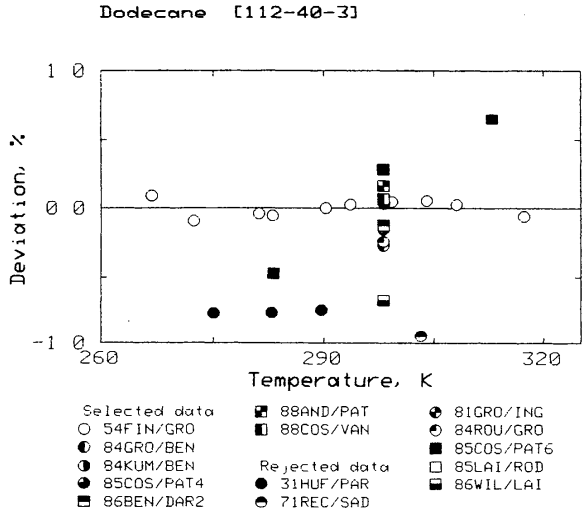

FIG. 12. Deviation plot for dodecane.

Table 37. Experimental heat capacities for tridecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
54FIN/GRO *N*	271.7–306.4	8	0.20	99.95 melpt	C_{sat}	AD–43 RUE/HUF
75WOY/KAL	303.1	1	nosp	99.97 chrom	C_p	IP–70REC
76MUS	307.8–478.6	16	2.50	not specified	C_p	AD–71MUS

54FIN/GRO smoothed data in 67MES/GUT.

Table 38. Correlated heat capacities for tridecane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
54FIN/GRO	271.7–306.4	8	0.20	0.200	1.92–2	0.04	6.82–5	− 2
75WOY/KAL	303.1	1	0.50#	0.011	2.59–3	0.01	− 2.59–3	0

Table 39. Parameters of regression polynomial for tridecane.

			Statistics				
Heat cap. type	No. points total	No. points used	s_w	s/R	S_r %	s_b/R	+/−
C	25	9	0.231	2.23–2	0.05	− 2.27–4	− 2
			Parameters				
Temp range K		A_0	A_1		A_2		Level of accuracy
271.7–306.4		9.315 35 + 1	− 3.592 70 + 1		7.073 13		II

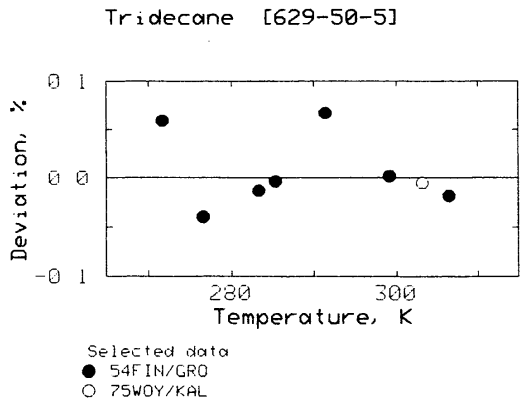

FIG. 13. Deviation plot for tridecane.

Table 40. Experimental heat capacities for tetradecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
34PAR/LIG	280.6–290.6	4	1.00	not specified	C_p	IP–25PAR
54FIN/GRO *N*	282.7–302.8	7	0.20	99.93 melpt	C_{sat}	AD–43RUE/HUF
76MUS	307.8–501.5	18	2.50	not specified	C_p	AD–71MUS
84GRI/AND	296.2–433.3	8	0.80	not specified	C_p	AD–67RAS/GAN
84GRO/BEN	298.1	1	nosp	99.5 estim	C_p	FL–71PIC/LED
84GRO/ING	298.1	1	nosp	99.0 estim	C_p	FL–71PIC/LED
84ROU/GRO	298.1	1	nosp	99.0 estim	C_p	FL–71PIC/LED
85BAL/BRA	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
85LAI/WIL	298.1	1	0.30	99.5 estim	C_p	FL–71PIC/LED
86WIL/LAI	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
87WIL/ING	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
88COS/VAN	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT.

Table 41. Correlated heat capacities for tetradecane.

Reference	Temp.range K	No. points used	$\sigma_R C^1$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
54FIN/GRO	282.7–302.8	7	0.20	0.158	1.67–2	0.03	8.89–3	3
84GRI/AND	296.2–433.3	8	0.80	0.345	1.53–1	0.28	− 5.64–2	0
84ROU/GRO	298.1	1	0.50#	0.648	1.70–1	0.32	− 1.70–1	− 1
88COS/VAN	298.1	1	0.50#	0.144	3.79–2	0.07	− 3.79–2	− 1

	Rejected data		
34PAR/LIG	(9.71–2, 0.91, − 9.69–2, − 3)	76MUS	(5.82, 10.99, − 5.74, − 11)
84GRO/BEN	(2.31–1, 0.44, − 2.31–1, − 1)	84GRO/ING	(2.17–1, 0.41, − 2.17–1, − 1)
85BAL/BRA	(5.77–1, 1.11, − 5.77–1, − 1)	85LAI/WIL	(4.96–1, 0.95, − 4.96–1, − 1)
86WIL/LAI	(5.23–1, 1.00, − 5.23–1, − 1)	87WIL/ING	(5.01–1, 0.96, − 5.01–1, − 1)

Table 42. Parameters of cubic spline polynomials for tetradecane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_b/R	+/−
C	45	17	0.362	1.36–1	0.25	− 3.52–2	1

Temp. range K	Parameters A_0	A_1	A_2	A_3	Level of accuracy
282.71–298.50	− 1.029 10 + 2	1.549 46 + 2	− 5.325 16 + 1	6.302 12	II
298.50–433.26	9.251 08 + 1	− 4.145 64 + 1	1.254 50 + 1	− 1.045 35	IV

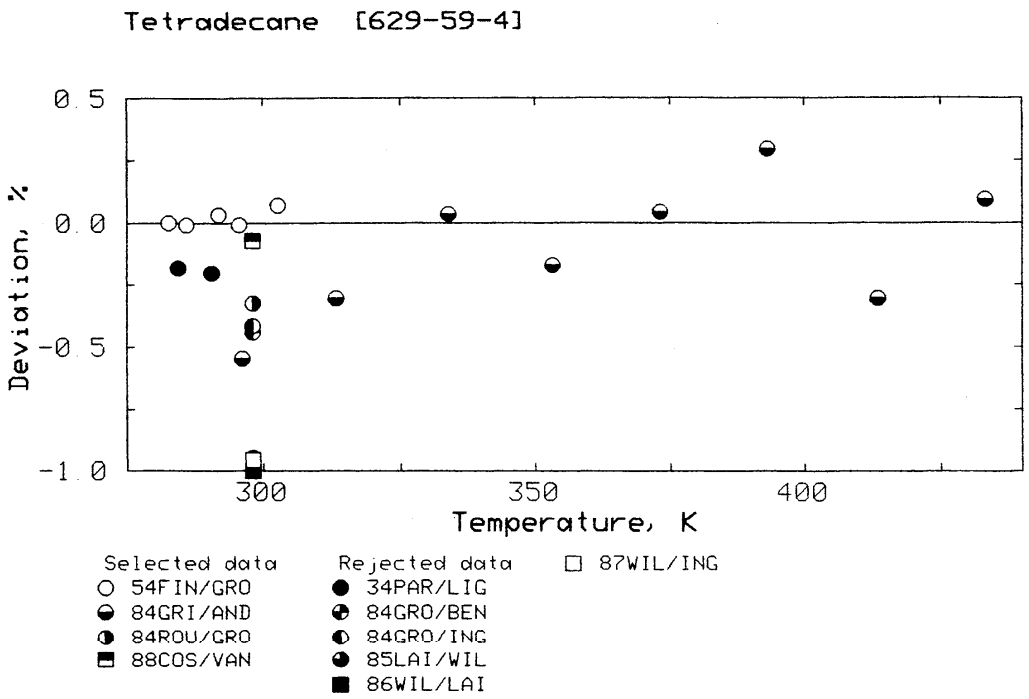

FIG. 14. Deviation plot for tetradecane.

Table 43. Experimental heat capacities for pentadecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
54FIN/GRO *N*	285.5–312.8	7	0.20	99.95 melpt	C_{sat}	AD–43RUE/HUF
70AKH	293.1	1	nosp	not specified	C_p	CC–59ABA/MUS
81GRO/ING	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
81COS/VAN	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT.

Table 44. Correlated heat capacities for pentadecane.

Reference	Temp.range K	No. points used	$\sigma_R C'$ %	d_w	d/R	d_r %	d_b/R	+/−
					Selected data			
54FIN/GRO	285.5–312.8	7	0.20	0.076	8.57–3	0.02	− 1.81–6	− 1
					Rejected data			
70AKH	(7.12–1, 1.25, 7.12–1, 1)				81GRO/ING	(2.58–1, 0.46, − 2.58–1, − 1)		
88COS/VAN	(1.37–1, 0.24, − 1.37–1, − 1)							

Table 45. Parameters of regression polynomial for pentadecane.

Heat cap. type	No. points total	No. points used	Statistics s_w	s/R	s_r %	s_h/R	+/−
C	10	7	0.101	1.13–2	0.02	− 1.81–6	− 1

Temp. range K	Parameters A_0	A_1	A_2	Level of accuracy
285.5–312.8	1.028 02 + 2	− 3.658 80 + 1	7.065 59	II

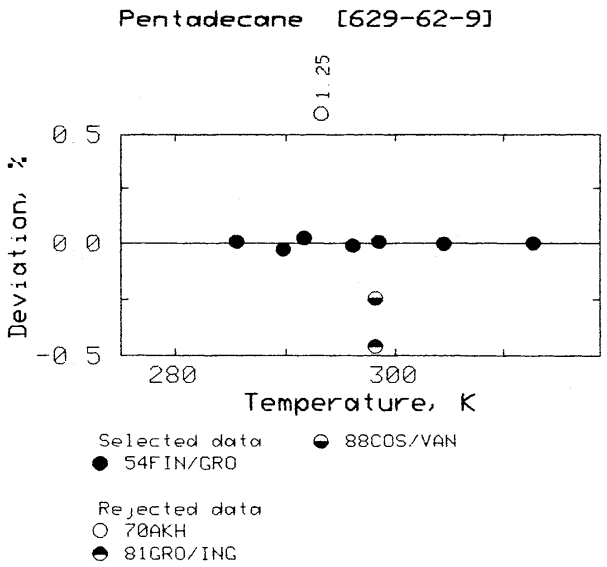

FIG. 15. Deviation plot for pentadecane.

Table 46. Experimental heat capacities for hexadecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
49PAR/MOO	L290.0–300.0	2S	1.00	95.0 estim	C_p	IP–25PAR
54FIN/GRO *N*	295.4–320.3	9	0.20	99.88 melpt	C_{sat}	AD–43RUE/HUF
56SCH/GOT	292.1–294.6	4	2.00	not specified	C_p	AD–33SOU/BRI
62GOL/BEL	310.9–422.0	3	nosp	96.9 chrom	C_p	DC–63GUD/CAM
68REC1 *N*	298.0–313.0	Eq.	nosp	not specified	C_p	AD–64REC1
70AKH	293.1	1	nosp	not specified	C_p	CC–59ABA/MUS
71REC/SAD	303.1	1	0.30	not specified	C_p	IP–70REC
72REC/SAD	298.1	1	0.30	not specified	C_p	IP–70REC
73KAL/WOY	303.1	1	0.20	99.5 chrom	C_p	IP–70REC
74DIA/REN	300.1–323.5	9	0.30	not specified	C_p	AD–74DIA/REN
74PET/TER	297.8–453.5	14	1.00	98.0 melpt	C_p	CT–74PET/TER
81GRO/ING	298.1	1	nosp	not specified	C_p	FL–71PIC/LED
85COS/PAT5	298.2	1	nosp	99.0 anal	C_p	FL–71PIC/LED
86WIL/LAI	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED
88COS/VAN	298.1	1	nosp	99.0 anal	C_p	FL–71PIC/LED

54FIN/GRO smoothed data in 67MES/GUT.
68REC1 the same data in 68REC2.

Table 47. Correlated heat capacities for hexadecane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
54FIN/GRO	295.4–320.3	9	0.20	0.209	2.58–2	0.04	8.09–3	−1
70AKH	293.1	1	0.50#	0.332	1.00–1	0.17	1.00–1	1
73KAL/WOY	303.1	1	0.20	0.480	583–2	0.10	5.83–2	1
74DIA/REN	300.1–323.5	9	0.30	0.586	1.08–1	0.18	6.47–3	3
74PET/TER	297.8–412.8	12	1.00	0.778	4.84–1	0.78	−1.93–1	−4
88COS/VAN	298.1	1	0.30#	0.930	1.68–1	0.28	−1.68–1	−1

Rejected data

49PAR/MOO	(3.01 − 1, 0.49, 3.01 − 1, 1)	56SCH/GOT	(3.30, 5.20, 3.30, 2)
62GOL/BEL	(2.54, 4.21, −2.52, −2)	68REC1	(2.03 − 1, 0.33, −1.90 − 1, −4)
71REC/SAD	(6.73 − 1, 1.12, −6.73 − 1, −1)	72REC/SAD	(6.02 − 1, 1.01, −6.02 − 1, −1)
81GRO/ING	(1.97 − 1, 0.33, −1.97 − 1, −1)	85COS/PAT5	(2.42 − 1, 0.40, −2.42 − 1, −1)
86WIL/LAI	(7.07 − 1, 1.18, −7.07 − 1, −1)		

Table 48. Parameters of cubic spline polynomials for hexadecane.

Heat cap. type	No. points total	No. points used	s_w	s/R	s_r %	s_b/R	+/−
		Statistics					
C	53	33	0.654	3.25–1	0.52	−6.64–2	−1

Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
	Parameters				
293.15–340.00	2.463 48 + 2	−1.760 84 + 2	5.345 27 + 1	−5.138 34	II
340.00–412.84	2.322 71 + 2	−1.636 62 + 2	4.979 95 + 1	−4.780 17	V

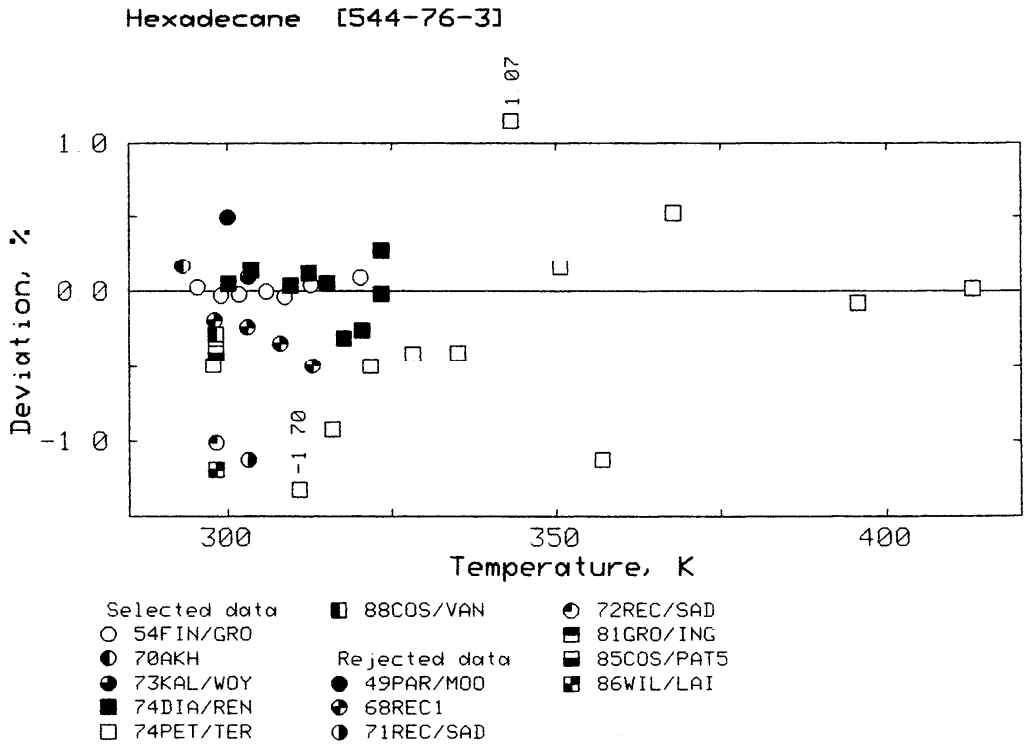

FIG. 16. Deviation plot for hexadecane.

Table 49. Experimental heat capacities for heptadecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
67MES/GUT	301.9–384.4	11	0.10	99.89 melpt	C_{sat}	AD–47HUF
70AKH	293.1	1	nosp	not specified	C_p	CC–59ABA/MUS

Table 50. Parameters of regression polynomial for heptadecane.

		Statistics					
Heat cap. type	No. points total	No. points used	s_w	s/R	s_r %	s_b/R	+/−
C	12	11	0.714	4.78–2	0.07	4.56–5	1

	Parameters			
Temp. range K	A_0	A_1	A_2	Level of accuracy
301.9–384.4	5.771 70 + 1	− 3.133 89	1.769 32	II

Table 51. Experimental heat capacities for octadecane.

Reference	Temp. range K	No. points	Error %	Purity % method	Type cap.	Calorimeter type-reference
49PAR/MOO	300.0	1	1.00	96.0 estim	C_p	IP–25PAR
67MES/GUT	304.4–378.7	11	0.10	99.98 melt	C_{sat}	AD–47HUF
81HOE	325.0–375.0	3S	5.00	not specified	C_p	DS–69PER/COM

Table 52. Correlated heat capacities for octadecane.

Reference	Temp. range K	No. points used	$\sigma_r C^l$	d_w	d/R	d_r %	d_b/R	+/−
			Selected data					
49PAR/MOO	300.0	1	1.00	0.270	1.83–1	0.27	− 1.83–1	− 1
67MES/GUT	304.4–378.7	11	0.10	0.521	3.72–2	0.05	1.99–4	0
			Rejected data					
81HOE	(2.34, 3.38, − 2.33, − 3)							

Table 53. Parameters of regression polynomial for octadecane.

		Statistics					
Heat cap. type	No. points total	No. points used	s_w	s/R	s_r %	s_b/R	+/−
C	15	12	0.583	7.36–2	0.11	− 1.51–2	− 1

	Parameters			
Temp. range K	A_0	A_1	A_2	Level of accuracy
300.0–378.7	6.533 47 + 1	− 5.632 31	2.180 35	II

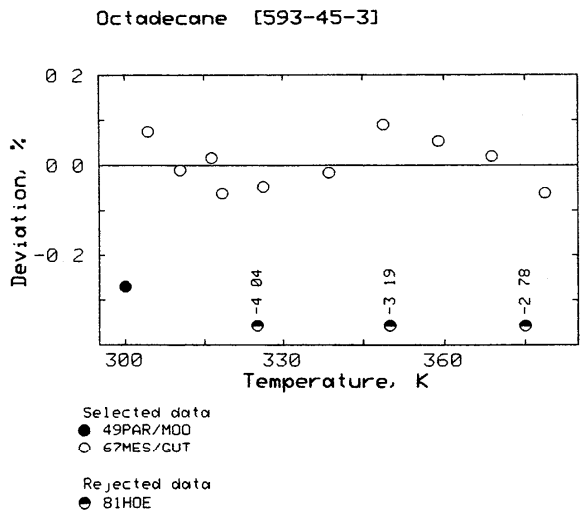

FIG. 17. Deviation plot for octadecane.

Table 54. Recommended values of heat capacities.

T/K	Methane		Ethane		Propane		Butane	
	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}
				$J\,K^{-1}\,mol^{-1}$				
90					84.08	84.08		
100	54.09	54.02	68.54	68.53	84.63	84.63		
110	55.28	55.22	68.84	68.82	85.26	85.25		
120	56.68	56.56	69.06	69.05	85.91	85.91		
130	58.74	58.24	69.28	69.28	86.59	86.59		
140	61.45	60.32	69.58	69.58	87.31	87.31	113.45	113.45
150	64.71	62.85	70.05	70.05	88.09	88.09	114.65	114.64
160	69.6	66.6	70.74	70.73	88.94	88.94	115.69	115.69
170	81.9	75.1	71.66	71.61	89.90	89.89	116.65	116.65
180	108.6	92.6	72.80	72.66	90.96	90.96	117.58	117.58
190			74.15	73.90	92.16	92.15	118.53	118.53
200			75.68	75.30	93.51	93.49	119.57	119.58
210			77.40	76.87	95.03	94.99	120.76	120.77
220			79.28	78.58	96.75	96.67	122.2	122.2
230			81.4	80.5	98.67	98.54	123.8	123.8
240			84.5	83.1	100.84	100.61	125.6	125.6
250			89.1	86.8	103.26	102.90	127.7	127.7
260			96.1	92.0	105.95	105.41	130.1	130.0
270			106.1	99.3	108.95	108.16	132.7	132.5
273.15			110.0	102.1	109.96	109.08	133.6	133.4
280			119.8	109.1	112.27	111.17	135.5	135.3
290			141.1	123.7			138.7	138.3
298.15			210.9	166.0			141.4	140.9
300			241.9	184.4			142.1	141.5
310							145.7	145.0
320							149.8	148.9
330							154.5	153.2
340							160.0	158.3
350							166.7	164.2
360							174.7	171.1

T/K	Pentane		Hexane		Heptane		Octane	
	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}
				$J\,K^{-1}\,mol^{-1}$				
150	141.58	141.58						
160	141.61	141.61						
170	141.91	141.91						
180	142.46	142.46						
190	143.28	143.27	170.61	170.61	201.81	201.81		
200	144.35	144.35	171.33	171.33	201.30	201.30		
210	145.70	145.69	172.55	172.55	201.62	201.61		

Table 54. Recommended values of heat capacities—Continued

T/K	Pentane		Hexane		Heptane		Octane	
	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}
				$J\,K^{-1}\,mol^{-1}$				
220	147.30	147.30	174.21	174.21	202.65	202.64		
230	149.16	149.16	176.22	176.22	204.29	204.29	233.41	233.41
240	151.24	151.25	178.52	178.52	206.45	106.45	235.14	235.14
250	153.56	153.56	181.04	181.04	209.01	209.01	237.46	237.46
260	156.07	156.07	183.73	183.73	211.88	211.89	240.30	240.30
270	158.78	158.76	186.59	186.59	214.97	214.98	243.59	243.59
273.15	159.67	159.65	187.52	187.53	215.98	215.99	244.70	244.70
280	161.67	161.62	189.62	189.62	218.26	218.27	247.24	247.24
290	164.71	164.62	192.85	192.84	221.73	221.74	251.18	251.18
298.15	167.31	167.17	195.63	195.62	224.70	224.71	254.55	254.55
300	167.9	167.8	196.28	196.27	225.40	225.40	255.33	255.34
310	171.3	171.0	199.94	199.91	229.24	229.22	259.64	259.64
320	174.8	174.4	203.82	203.77	233.25	233.21	264.08	264.09
330	178.5	178.0	207.96	207.88	237.43	237.36	268.66	268.67
340	182.3	181.6	212.4	212.2	241.77	241.66	273.38	273.38
350	186.4	185.4	217.0	216.8	246.26	246.10	278.23	278.22
360	190.6	189.3	221.8	221.5	250.90	250.68	283.22	283.18
370	195.0	193.4	226.7	226.2	255.69	255.38	288.35	288.26
380	199.6	197.6	231.8	231.0	260.60	260.20	293.62	293.47
390	204.4	201.9	236.9	235.8	265.65	265.14	299.02	298.78
400			242.1	240.5	270.82	270.18	304.56	304.21
410			247.2	245.0	276.13	275.33	310.24	309.75
420			252.4	249.4	281.64	280.62	316.05	315.40
430			257.4	253.5	287.47	286.10	322.00	321.15
440			262.3	257.3	293.71	291.83	328.09	327.00
450			267.1	260.7	300.45	297.84	334.32	332.95
460			271.7	263.7	307.80	304.20	340.68	338.99
470					315.84	310.93		
480					324.69	318.10		
490					334.42	325.75		
500					346.56	334.94		
510					368.24	350.73		
520					408.01	379.22		

T/K	Nonane	Decane		Undecane	Dodecane
	C	C_p	C_{sat}	C	C
		$J\,K^{-1}\,mol^{-1}$			
230	264.49				
240	265.25				
250	267.00	297.47	297.47		
260	269.58	299.87	299.87	330.94	
270	272.84	302.95	302.95	333.45	364.62
273.15	273.99	304.04	304.04	334.47	365.63
280	276.64	306.61	306.61	336.98	368.04
290	280.83	310.75	310.75	341.19	372.09
298.15	284.43	314.43	314.42	344.94	375.84
300	285.26	315.29	315.29	345.8	376.75
310	289.79	320.13	320.13	350.8	382.02
320		325.19	325.19	356.0	
330		330.41	330.42	361.6	
340		335.81	335.82	367.3	
350		341.38	341.39	373.2	
360		347.12	347.12	379.2	
370		353.03	353.02	385.4	
380		359.11	359.09	391.6	
390		365.36	365.32	397.8	
400		371.78	371.70	404.0	
410		378.38	378.25	410.1	
420		385.14	384.95	416.2	
430		392.07	391.80	422.1	
440		399.18	398.81		
450		406.45	405.97		
460		413.90	413.28		

Table 54. Continued

T/K	Tridecane	Tetradecane	Pentadecane	Hexadecane	Heptadecane	Octadecane
	C	C	C $J\,K^{-1}\,mol^{-1}$	C	C	C
273.15	397.36					
280	399.18					
290	402.83	434.76	466.59			
298.15	406.68	438.33	469.95	501.61		
300	407.66	439.2	470.82	502.49		565.88
310		444.1	476.21	507.95	540.47	572.26
320		449.4		514.36	547.14	578.99
330		455.2		521.44	554.09	586.09
340		461.4		528.96	561.34	593.56
350		467.8		536.7	568.89	601.38
360		474.6		544.3	576.73	609.57
370		481.5		551.6	584.86	618.12
380		488.6		558.4	593.29	
390		495.8		564.4		
400		503.0		569.4		
410		510.3		573.1		
420		517.5				
430		524.6				
440						
450						
460						

Table 55. Parameters of quasipolynomial extrapolation equation.

	Methane	Ethane	Propane	Butane	Pentane
T_c/K	190.55	305.33	369.85	425.25	469.80
E_{-1}	2.659 62 − 1	3.127 22 − 1	8.605 16 − 1	5.966 20 − 1	2.542 74 − 1
E_0	9.334 97	1.169 87 + 1	1.087 70 + 1	1.999 43 + 1	2.606 11 + 1
E_1	− 2.276 87 + 1	− 1.808 41 + 1	− 4.288 47	− 2.068 93 + 1	− 1.756 45 + 1
E_2	6.022 55 + 1	3.241 80 + 1	2.569 70	1.884 30 + 1	1.268 22 + 1
E_3	− 2.168 43 + 2	− 1.068 68 + 2	− 1.781 00	− 5.978 80 + 1	− 1.011 08 + 2
E_4	1.288 96 + 3	4.686 67 + 2	3.201 60	1.633 57 + 2	2.190 13 + 2
E_5	− 4.124 94 + 3	− 1.014 24 + 3	− 1.534 75	− 1.190 23 + 2	− 1.265 09 + 2
E_6	6.160 43 + 3	1.022 17 + 3			
E_7	− 3.577 87 + 3	− 3.997 42 + 2			
s/R	2.47–1	1.84–1	3.06–2	2.80–1	1.47–1
Level of accuracy	V	V	III	V	IV

	Hexane	Heptane	Octane	Nonane	Decane
T_c/K	507.90	540.15	568.95	594.90	617.65
E_{-1}	5.822 33 − 1	4.011 68 − 1	2.878 21 − 1	1.504 71 + 2	1.692 61 − 1
E_0	3.213 49 + 1	3.842 98 + 1	4.462 15 + 1	− 1.332 69 + 3	5.712 68 + 1
E_1	− 2.651 89 + 1	− 2.747 00 + 1	− 2.602 13 + 1	4.126 45 + 3	− 2.533 17 + 1
E_2	1.896 28 + 1	1.961 10 + 1	1.732 89 + 1	− 2.646 35 + 3	1.684 56 + 1
E_3	− 1.006 54 + 2	− 1.567 50 + 2	− 1.960 44 + 2	− 9.430 17 + 3	− 3.159 29 + 2
E_4	2.159 24 + 2	3.357 16 + 2	3.916 68 + 2	1.814 31 + 4	6.302 78 + 2
E_5	− 1.235 20 + 2	− 1.917 36 + 2	− 2.086 66 + 2	− 9.308 34 + 3	− 3.353 08 + 2
s/R	4.26–1	1.14–1	1.43–1	3.87–2	1.24–1
Level of accuracy	V	III	III	III	III

	Undecane	Dodecane	Tetradecane	Hexadecane	Heptadecane
T_c/K	638.85	658.65	693.00	722.00	735.00
E_{-1}	2.736 94	1.587 64 + 2	6.317 94	4.874 29 + 2	8.047 97 + 1
E_0	1.063 07 + 1	− 1.398 23 + 3	− 2.019 28 + 1	− 4.214 34 + 3	− 7.052 83 + 2

Table 55. Continued

	Undecane	Dodecane	Tetradecane	Hexadecane	Heptadecane
E_1	2.008 85 + 2	4.362 75 + 3	3.790 82 + 2	1.251 17 + 4	2.467 72 + 3
E_2	− 1.360 38 + 2	− 2.754 29 + 3	− 2.535 65 + 2	− 7.873 76 + 3	− 1.521 03 + 3
E_3	− 1.228 70 + 3	− 9.990 54 + 3	− 1.895 44 + 3	− 2.676 35 + 4	− 6.305 56 + 3
E_4	2.496 22 + 3	1.892 17 + 4	3.803 53 + 3	5.052 76 + 4	1.165 97 + 4
E_5	− 1.352 34 + 3	− 9.556 51 + 3	− 2.035 33 + 3	− 2.543 80 + 4	− 5.749 37 + 3
s/R	9.74–2	4.32–2	1.51–1	3.11–1	1.78–2
Level of accuracy	IV	III	IV	IV	III

	Octadecane
T_c/K	746.00
E_{-1}	1.236 05 + 2
E_0	− 1.076 62 + 3
E_1	3.537 98 + 3
E_2	− 2.167 28 + 3
E_3	− 8.439 06 + 3
E_4	1.550 87 + 4
E_5	− 7.600 17 + 3
s/R	9.87–2
Level of accuracy	III

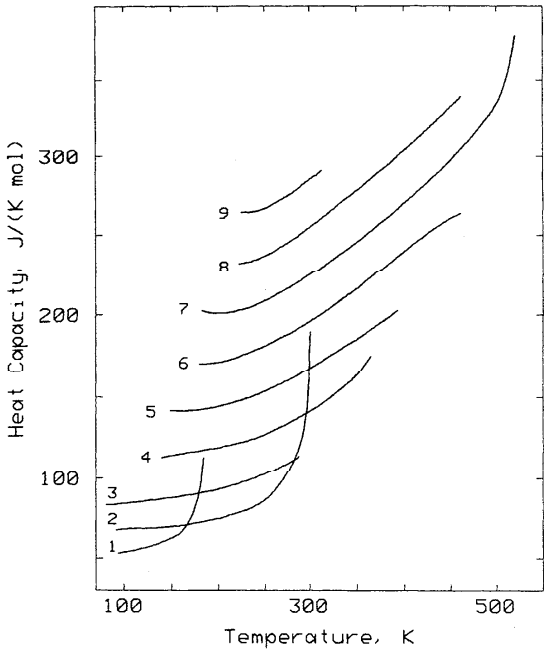

FIG. 18. Temperature dependence of saturation heat capacity for C_1 to C_9 n-alkanes.

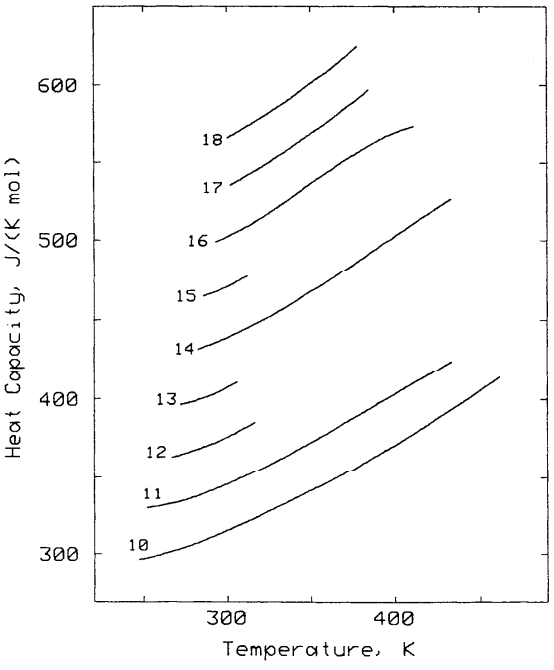

FIG. 19. Temperature dependence of saturation heat capacity for C_{10} to C_{18} n-alkanes.

Table 56. Comparison with the DIPPR data.

	Temp. range K	Ave. dif. %	Max. Dif. %	Ave. ratio	Max. ratio
			n-Alkanes		
C_1	93–180	0.85	1.73	0.15	0.31
C_2	90–290	0.85	− 1.60	0.15	0.29
C_3	90–288	0.48	1.00	0.14	0.31
C_4	140–160	0.90	3.05	0.22	0.87
C_5	150–300	0.19	− 0.53	0.04	0.10
C_6	180–360	0.24	0.57	0.07	0.16
C_7	183–520	0.58	− 2.61	0.18	0.80
C_8	222–390	0.65	− 1.86	0.19	0.53
C_9	225–314	0.11	− 0.18	0.03	0.06
C_{10}	247–330	0.21	− 0.57	0.06	0.17
C_{11}	252–330	0.17	− 1.11	0.04	0.28
C_{12}	267–317	0.02	0.04	0.01	0.01
C_{13}	272–306	0.03	0.06	0.03	0.05
C_{14}	283–310	0.03	0.09	0.02	0.04
C_{15}	285–313	0.00	− 0.01	0.00	0.01
C_{16}	293–330	0.07	0.24	0.06	0.19
			1-Alkanols		
C_1	180–370	0.42	0.95	0.34	0.64
C_2	160–370	0.37	− 0.89	0.07	0.17
C_3	160–450	3.94	21.83	1.10	5.46
C_4	200–320	0.14	0.35	0.03	0.06
C_5	210–380	0.78	− 1.38	0.25	0.44
C_6	230–290	0.97	− 1.71	0.24	0.43

6. Acknowledgments

The authors thank Drs. E. S. Domalski and K. N. Marsh for helpful comments and Dr. K. Kollár-Hunek for providing the routine for weighted least-squares fitting by cubic splines. One of the authors (V.M.) acknowledges the support of the Office of Standard Reference Data of the National Institute of Standards and Technology (Grant no. 60NANB9DO912). The authors thank the Thermodynamic Research Center, Texas A&M University for donation of the TRC tables.

7. References

24EUC/KAR Eucken, A., Karwat, E., Z. Phys. Chem. Stoechiom. Verwandtschaftslehre **112**, 467–85 (1924).
24WIL/DAN Williams, J. W., Daniels, F., J. Am. Chem. Soc. **46**, 903–17 (1924).
25PAR Parks, G. S., J. Am. Chem. Soc. **47**, 338–45 (1925).
26DAN/JEN Dana, L. I., Jenkins, A. C., Burdick, J. N., Timm, R. C., Refrig. Eng. **12**, 387–405 (1926).
28EUC/HAU Eucken, A., Hauck, F., Z. Phys. Chem. Stoechiom. Verwandtschaftslehre **134**, 161–77 (1928).
28GIA/WIE Giauque, W. F., Wiebe, R., J. Am. Chem. Soc. **50**, 101–22 (1928).
28LAT/GRE Latimer, W. M., Greensfelder, B. S., J. Am. Chem. Soc. **50**, 2202–13 (1928).
29CLU Clusius, K., Z. Phys. Chem. B **3**, 41–79 (1929).
30PAR/HUF1 Parks, G. S., Huffman, H. M., J. Am. Chem. Soc. **52**, 4381–91 (1930).
30PAR/HUF2 Parks, G. S., Huffman, H. M., Thomas, S. B., J. Am. Chem. Soc. **52**, 1032–41 (1930).
30WIE/BRE Wiebe, R., Brevoort, M. J., J. Am. Chem. Soc. **52**, 622–33 (1930).
30WIE/HUB Wiebe, R., Hubbard, K. H., Brevoort, M. J., J. Am. Chem. Soc. **52**, 611–22 (1930).
31HUF/PAR Huffman, H. M., Parks, G. S., Barmore, M., J. Am. Chem. Soc. **53**, 3876–88 (1931).
33SOU/BRI Southard, J. C., Brickwedde, F. G., J. Am. Chem. Soc. **55**, 4378–84 (1933).
34PAR/LIG Parks, G. S., Light, D. W., J. Am. Chem. Soc. **56**, 1511–3 (1934).
35SAG/LAC Sage, B. H., Lacey, W. N., Ind. Eng. Chem. **27**, 1484–8 (1935).
36AST/MES Aston, J. G., Messerly, G. H., J. Am. Chem. Soc. **58**, 2354–61 (1936).
37STU Stull, D. R., J. Am. Chem. Soc. **59**, 2726–33 (1937).
37VOL Vold, R. D., J. Am. Chem. Soc. **59**, 1515–21 (1937).
37WIT/KEM Witt, R. K., Kemp. J. D., J. Am. Chem. Soc. **59**, 273–6 (1937).
38KEM/EGA Kemp, J. D., Egan, C. J., J. Am. Chem. Soc. **60**, 1521–5 (1938).
39BYK Bykov, V. T., Zh. Fiz. Khim. **13**, 1013–9 (1939).
39PHI Philip, N. M., Proc. Indian Acad. Sci. Sec. A **9**, 109–20 (1939).
39SAG/EVA Sage, B. H., Evans, H. D., Lacey, W. N., Ind. Eng. Chem. **31**, 763–7 (1939).
40AST/MES Aston, J. G., Messerly, G. H., J. Am. Chem. Soc. **62**, 1917–23 (1940).
40MES/KEN Messerly, G. H., Kennedy, R. M., J. Am. Chem. Soc. **62**, 2988–91 (1940).
40PIT Pitzer, K. S., J. Am. Chem. Soc. **62**, 1224–7 (1940).
43RUE/HUF Ruehrwein, R. A., Huffman, H. M., J. Am. Chem. Soc. **65**, 1620–5 (1943).
45SCO/MEY Scott, R. B., Meyers, C. H., Rands, R. D., Jr., Brickwedde, F. G., Bekkedahl, N., J. Res. Natl. Bur. Std. (U.S.) **35**, 39–85 (1945).
46DOU/HUF Douslin, D. R., Huffman, H. M., J. Am. Chem. Soc. **68**, 1704–8 (1946).
47HUF Huffman, H. M., Chem. Rev. **40**, 1–14 (1947).
47OSB/GIN Osborne, N. S., Ginnings, D. C., J. Res. Natl. Bur. Std. (U.S.) **39**, 453–77 (1947).
49PAR/MOO Parks, G. S., Moore, G. E., Renquist, M. L., Naylor, B. F., McClaine, L. A., Fujii, P. S., Hatton, J. A., J. Am. Chem. Soc. **71**, 3386–9 (1949).
49TSC/RIC Tschamler, H., Richter, E., Monatsch. Chem. **80**, 510–6 (1949).
49TSC/WET Tschamler, H., Wettig, F., Richter, E., Monatsh. Chem. **80**, 572–82 (1949).
49WEI Weissberger, A. (editor), Physical Methods of Organic Chemistry, Interscience Publ. Co., New York 1/1, 773 (1949).

50GIN/DOU Ginnings, D. C., Douglas, T. B., Ball, A. F., J. Res. Natl. Bur. Std. (U.S.) **45**, 23–33 (1950).
51CON/SAG Connolly, T. J., Sage, B. H., Lacey, W. N., Ind. Eng. Chem. **43**, 946–50 (1951).
52SCH/SAG Schlinger, W. G., Sage, B. H., Ind. Eng. Chem. **44**, 2454–6 (1952).
53GIN/FUR Ginnings, D. C., Furukawa, G. T., J. Am. Chem. Soc. **75**, 522–7 (1953).
53RIF/KER Rifkin, E. B., Kerr, E. C., Johnston, H. L., J. Am. Chem. Soc. **75**, 785–8 (1953).
54DOU/FUR Douglas, T. B., Furukawa, G. T., McCoskey, R. E., Ball, A. F., J. Res. Natl. Bur. Std. (U.S.) **53**, 139–53 (1954).
54FIN/GRO Finke, H. L., Gross, M. E., Waddington, G., Huffman, H. M., J. Am. Chem. Soc. **76**, 333–41 (1954).
56SCH/GOT Schrock, V. E., Gott, R. E., Starkman, E. S., WADC Technical Report 56–104, 1–144 (1956).
58SWI/ZIE Swietoslawski, W., Zielenkiewicz, A., Bull. Acad. Pol. Sci., Ser. Sci. Chim. Geol. Geogr. **6**, 365–6 (1958).
59ABA/MUS Abas-Zade, A. K., Mustafaev, R. A., Dokl. Akad. Nauk. Azerb, SSR **15**, 775–9 (1959).
61FLU/LEA Flubacher, P., Leadbetter, A. J., Morrison, J. A., Proc. Phys. Soc., London **78**, 1149–61 (1961).
61GOO Goodwin, R. D., J. Res. Natl. Bur. Std. (U.S.) **65C**, 231–43 (1961).
61HES/WHI Hestermans, P., White, D., J. Phys. Chem. **65**, 362–5 (1961).
61HUF/GRO Huffman, H. M., Gross, M. E., Scott, D. W., McCullough, J. P., J. Phys. Chem. **65**, 495–503 (1961).
61MCC/MES McCullough, J. P., Messerly, J. F., U.S. Bur. Mines Bull. **596**, 1–15 (1961).
61ROU Rousseau, R. A., Ph.D. Thesis, John Hopkins University, Baltimore, Maryland (1961).
62GOL/BEL Gollis, M. H., Belenyessy, L. I., Gudzinowicz, B. J., Koch, S. D., Smith, J. O., Wineman, R. J., J. Chem. Eng. Data **7**, 311–6 (1962).
63COL/GIL Colwell, J. H., Gill, E. K., Morrison, J. A., J. Chem. Phys. **39**, 635–53 (1963).
63GUD/CAM Gudzinowicz, B. J., Campbell, R. H., Adamas, J. S., J. Chem. Eng. Data **8**, 201–4 (1963).
65CUT/MOR Cutler, A. J. B., Morrison, J. A., Trans. Faraday Soc. **61**, 429–42 (1965).
65FIN/GRU Findenegg, G. H., Gruber, K., Pereira, J. F., Kohler, F., Monatsh. Chem. **96**, 669–78 (1965).
66KLE Klesper, I., Z. Phys. Chem. (Frankfurt am. Main) **51**, 1–12 (1966).
67MES/GUT Messerly, J. F., Guthrie, G. B., Todd, S. S., Finke, H. L., J. Chem. Eng. Data **12**, 338–46 (1967).
67RAS/GAN Rastorguev, Yu. L., Ganiev, Yu. A., Izv. Vyssh. Ucheb. Zaved., Neft Gas **10**(1), 79–82 (1967).
68REC1 Recko, W. M., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **16**, 543–8 (1968).
68REC2 Recko, W. M., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **16**, 553–5 (1968).
69PER/COM Perkin-Elmer DSC-2, commercial calorimeter, Prospectus (1969).
69WIL/ROT Wilhelm, E., Rott, E., Kohler, F., Proc. 1st Intern. Conf. Calorimetry and Thermodynamics, Warszaw 767–71 (1969).
70AKH Akhmedov, A. G., Zh. Fiz. Khim. **44**, 2061–2 (1970).
70REC Recko, W. M., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **18**, 297–301 (1970).
70TOU/MAK Touloukian, Y. S., Makita, T., Thermophysical Properties of Matter, Vol. 6, Specific Heats of Nonmetallic Liquids and Gases, IFI/Plenum, New York (1970).
71AMI/ALI Amirkhanov, Kh.I., Alibekov, B. G., Vikhrov, D. I., Mirskaya, V. A., Levina, L. N., Teplofiz. Vys. Temp. **9**, 1310–3 (1971).
71MUS Mustafaev, R. A., Izv. Vyssh. Ucheb. Zaved., Priborostr. **14**(7), 129–34 (1971).
71PIC/LED Picker, P., Leduc, P. A., Philip, P. R., Desnoyers, J. E., J. Chem. Thermodyn. **3**, 631–42 (1971).
71REC/SAD Recko, W. M., Sadowska, K. W., Woycicka, M. K., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **19**, 475–91 (1971).
72REC/SAD Recko, W. M., Sadowska, K. W., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **20**, 73–9 (1972).
72VAN Van Miltenburg, J. C., J. Chem. Thermodyn. **4**, 773–82 (1972).
73KAL/WOY Kalinowska, B., Woycicka, M., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **21**, 845–8 (1973).
74DIA/REN Diaz Pena, M., Renuncio, J. A. R., An. Quim. **70**, 113–20 (1974).
74PEN/STI Peng, D., Stiel, L. I., Thermodynamics-Data and Correlations, AIChE Symp. Ser. **70**(140), 63–9 (1974).
74PET/TER Petit, J. C., Ter Minassian, L., J. Chem. Thermodyn. **6**, 1139–52 (1974).
74YOU Younglove, B. A., J. Res. Natl. Bur. Std. (U.S.) **78A**, 401–10 (1974).
75GRI/RAS Grigor'ev, B. A., Rastorguev, Yu. L., Yanin, G. S., Izv. Vyssh. Ucheb. Zaved., Neft Gaz **18**(10), 63–6 (1975).
75HOL/ZIE Holzhauer, J. K., Ziegler, W. T., J. Phys. Chem. **79**, 590–604 (1975).
75RAS/GRI Rastorguev, Yu. L., Grigor'ev, B. A., Yanin, G. S., Izv. Vyssh. Ucheb. Zaved., Neft Gas **18**(4), 73–7 (1975).
75SAF/GER Safir, L. I., Gerasimov, A. A., Grigor'ev, B. A., Izv. Vyssh. Ucheb. Zaved., Neft Gaz **18**(11), 61–5 (1975).
75SAN San Jose, J. L., Ph.D. Thesis, Massachusetts Institute of Technology (1975).
75WOY/KAL Woycicka, M. K., Kalinowska, B., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **23**, 759–64 (1975).
76KAR/GRO Karbalai Ghassemi, M. H., Grolier, J.-P.E., Int. Data Ser., Sel. Data Mixtures, Ser. A (2), 95 (1976).
76MUS Mustafaev, R. A., Zh. Fiz. Khim. **50**, 1899 (1976), data deposited in VINITI 1224-76.
76ROD1 Roder, H. M., J. Chem. Phys. **65**, 1371–3 (1976).
76ROD2 Roder, H. M., J. Res. Natl. Bur. Std. (U.S.) **80A**, 739–59 (1976).
76TOU/MAK Touloukian, Y. S., Makita, T., Thermophysical Properties of Matter, Supplement to Vol. 6, Specific Heats of Nonmetallic Liquids and Gases, IFI/Plenum, New York (1976).
77ENG Heat Capacity and Enthalpy of Liquids: Alkanes, Engineering Science Data Item Number 77025, Engineering Science Data Unit London (1977).
77MEI/BLO Meijer, E. L., Blok, J. G., Kroon, J., Oonk, H. A. J., Thermochim. Acta **20**, 325–34 (1977).
77TEJ/SIN Teja, A. S., Singh, A., Cryogenics **17**, 591–6 (1977).
78GOO Goodwin, R. D., J. Res. Natl. Bur. Std. (U.S.) **83**, 449–58 (1978).
79BRO/ZIE Brown, G. N., Jr., Ziegler, W. T., J. Chem. Eng. Data **24**, 319–30 (1979).
79CZA Czarnota, I., Bull. Acad. Pol. Sci., Ser. Sci. Chim. **27**, 763–72 (1979).
79 GRO/HAM Grolier, J.-P. E., Hamedi, M. H., Wilhelm, E., Kehiaian, H. V., Thermochim. Acta **31**, 79–84 (1979).
79SCH/OFF Schaake, R. C. F., Offringa, J. C. A., Van der Berg, G. J. K., Van Miltenburg, J. C., Rec. Trav. Chim. Pays-Bas **98**, 408–12 (1979).
79VAN/ZEL Van Kasteren, P. H. G., Zeldenrust, H., Ind. Eng. Chem., Fundam. **18**, 339–45 (1979).
80KAL/JED Kalinowska, B., Jedlinska, J., Woycicki, W., Stecki, J., J. Chem. Thermodyn. **12**, 891–6 (1980).
80MIY/HEJ Miyazaki, T., Hejmadi, A. V., Powers, J. E., J. Chem. Thermodyn. **12**, 105–24 (1980).
80SHA/LYU Shakirov, R. F., Lyubarskii, M. V., deposited Doc. SPSTL 3Khp-D80, 1–19 (1980).
81GRO/ING Grolier, J.-P. E., Inglese, A., Roux, A. H., Wilhelm, E., Ber. Bunsenges. Phys. Chem. **85**, 768–72 (1981).
81HOE Hoehne, G. W. H., Polym. Bull. (Berlin) **6**, 41–6 (1981).
82WIL/ING Wilhelm, E., Inglese, A., Quint, J. R., Grolier, J.-P. E., J. Chem. Thermodyn. **14**, 303–8 (1982).
83ROU/ROU Roux, A. H., Roux-Desgranges, G., Grolier, J.-P. E., Viallard, A., Calorim. Anal. Therm. **14**, 142–50 (1983).
83SID/SVE Siddiqi, M. A., Svejda, P., Kohler, F., Ber. Bunsenges. Phys. Chem. **87**, 1176–81 (1983).
83TAN/ZHO Tan, Z., Zhou, L., Chen, S., Yin, A., Sun, Y., Ye, J., Wang, X., Sci. Sin., Ser. B **26**, 1014–26 (1983).
84BEN/DAR Benson, G. C., D'Arcy, P. J., Kumaran, M. K., Thermochim. Acta **75**, 353–60 (1984).
84BRA/PIN Bravo, R., Pintos, M., Baluja, M. C., Paz Andrade, M. I., Roux-Desgranges, G., Grolier, J.-P. E., J. Chem. Thermodyn. **16**, 73–9 (1984).
84COM IUPAC Commission on Atomic Weights and Abundances, Pure and Appl. Chem. **56**, 653 (1984).
84DOM/EVA Domalski, E. S., Evans, W. H., Hearing, E. D., J. Phys. Chem. Ref. Data **13**, 1–286 (1984), Supplement 1.
84GRI/AND Grigor'ev, B. A., Andolenko, R. A., Izv. Vyssh. Ucheb. Zaved., Neft Gaz **27**(2), 60–2 (1984).

84GRO/BEN Grolier, J.-P. E., Benson, G. C., Can. J. Chem. **62**, 949–53 (1984).
84GRO/ING Grolier, J.-P. E., Inglese, A., Wilhelm, E., J. Chem. Thermodyn. **16**, 67–71 (1984).
84GUS/MIR Guseinov, S. O., Mirzaliev, A. A., Izv. Vyssh. Ucheb. Zaved., Neft Gaz **27**(5), 41–5 (1984).
84KUM/BEN Kumaran, M. K., Benson, G. C., D'Arcy, P. J., Halpin, C. J., J. Chem. Thermodyn. **16**, 1181–9 (1984).
84ROU/GRO Roux, A. H., Grolier, J.-P. E., Inglese, A., Wilhelm, E., Ber. Bunsenges. Phys. Chem. **88**, 986–92 (1984).
85BAL/BRA Baluja, M. C., Bravo, R., Pintos, M., Paz Andrade, M. I., Roux-Desgranges, G., Grolier, J.-P. E., Calorim. Anal. Therm. **16**, 138–44 (1985).
85COS/PAT1 Costas, M., Patterson, D., Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 212 (1985).
85COS/PAT2 Costas, M., Patterson, D., Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 213 (1985).
85COS/PAT3 Costas, M., Patterson, D., Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 214 (1985).
85COS/PAT4 Costas, M., Patterson, D., Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 215 (1985).
85COS/PAT5 Costas, M., Patterson, D., Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 216 (1985).
85COS/PAT6 Costas, M., Patterson, D., J. Chem. Soc., Faraday Trans. 1 **81**, 635–54 (1985).
85CZA Czarnota, I., High Temp.–High Pressures **17**, 543–6 (1985).
85DIP DIPPR Data Compilation of Pure Compound Properties, NBS Standard Reference Data Base 11, Washington. D.C., Office of Standard Reference Data (updated periodically).
85GRI/GER Grigor'ev, B. A., Gerasimov, A. A., Kharin, V. E., Rastorguev, Yu. L., High Temp.–High Pressures **17**, 317–24 (1985).
85LAI/GRO Lainez, A., Grolier, J.-P. E., Wilhelm, E., Thermochim. Acta **91**, 243–8 (1985).
85LAI/ROD Lainez, A., Rodrigo, M., Roux, A. H., Grolier, J.-P. E., Wilhelm, E., Calorim. Anal. Therm. **16**, 153–8 (1985).
85LAI/WIL Lainez, A., Wilhelm E., Roux-Desgranges, G., Grolier, J.-P. E., J. Chem. Thermodyn. **17**, 1153–61 (1985).
85WIL/CHA Wilhoit, R. C., Chao, J., Hall, K. R., J. Phys. Chem. Ref. Data **14**, 1–175 (1985).
86BEN/DAR1 Benson, G. C., D'Arcy, P. J., Can. J. Chem. **64**, 2139–41 (1986).
86BEN/DAR2 Benson, G. C., D'Arcy, P. J., Thermochim. Acta **102**, 75–81 (1986).
86GAT/WOO Gates, J. A., Wood, R. H., Cobos, J. C., Casanova, C., Roux, A. H., Roux-Desgranges, G., Grolier, J.-P. E., Fluid Phase Equilib. **27**, 137–51 (1986).
86NAZ/BAS1 Naziev, Ya. M., Bashirov, M. M., Badalov, Yu. A., Inzh.–Fiz. Zh. **51**, 789–95 (1986).
86NAZ/BAS2 Naziev, Ya. M., Bashirov, M. M., Badalov, Yu. A., Inzh.–Fiz. Zh. **51**, 998–1004 (1986).
86WIL/LAI Wilhelm, E., Lainez, A., Roux, A. H., Grolier, J.-P. E., Thermochim. Acta **105**, 101–10 (1986).
87TRC TRC Thermodynamics Tables—Hydrocarbons, Thermodynamics Research Center, Texas A&M University System, College Station, Texas (1987).
87VAN/VAN Van Miltenburg, J. C., Van den Berg, J. K., Van Bommel, M. J., J. Chem. Thermodyn. **19**, 1129–37 (1987).
87WIL/ING Wilhelm, E., Inglese, A., Roux, A. H., Grolier, J.-P. E., Fluid Phase Equilib. **34**, 49–67 (1987).
88AND/PAT Andreoli-Ball, L., Patterson, D., Costas, M., Caceres-Alonso, M., J. Chem. Soc., Faraday Trans. 1 **84**, 3991–4012 (1988).
88COS/VAN Costas, M., Van Tra, H., Patterson, D., Caceros-Alonso, M., Tardajos, G., Aicart, E., J. Chem. Soc., Faraday Trans. 1 **84**, 1603–16 (1988).
88KUZ/KHA Kuznetsov, M. A., Kharin, V. E., Gerasimov, A. A., Grigor'ev, B. A., Izv. Vyssh. Ucheb. Zaved., Neft Gas **31**(11), 49–52 (1988).
88MAR Marsh, K. N. (Editor), Recommended Reference Materials for the Realization of Physicochemical Properties. IUPAC/Blackwell. Oxford, 1988.
88MEL/VER Mel'nikov, G. A., Verveiko, V. N., Otpushchennikov, N. F., Zh. Fiz. Khim. **62**, 799–800 (1988).
88PIN/BRA Pintos, M., Bravo, R., Baluja, M. C., Paz Andrade, M. I., Roux-Desgranges, G., Grolier, J.-P. E., Can. J. Chem. **66**, 1179–86 (1988).
88SAI/TAN Saito, A., Tanaka, R., J. Chem. Thermodyn. **20**, 859–65 (1988).
90ZAB/RUZ1 Zabransky, M., Ruzicka, V., Jr., Majer, V., Sb. Vys. Sk. Chemicko-Technol. Praze, Fyz. Chem. N**10**, 55–68 (1990).
90ZAB/RUZ2 Zabransky, M., Ruzicka, V., Jr., Majer, V., J. Phys. Chem. Ref. Data **19**, 719–762 (1990).