Heat Capacities and Entropies of Organic Compounds in the Condensed Phase Volume II

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This compilation of data on the heat capacities, entropies, and phase transitions of organic compounds in the condensed phase supplements the document published earlier on this subject, namely, "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase" by E. S. Domalski, W. H. Evans, and E. D. Hearing, J. Phys. Chem. Ref. Data, **13**, Suppl. 1, (1984). It provides data on approximately 1300 organic compounds. About half of the articles examined contain data published prior to 1982. A total of 565 articles have been examined, evaluated, and referenced. In addition to values for the heat capacity and entropy at 298.15 K, phase transitions for solid/solid, solid/liquid, and in some instances, solid/gas and liquid/gas are tabulated as encountered from the articles examined and evaluated.

Key words: condensed phase; entropy; evaluated data; heat capacity; organic compounds; phase transitions; WLN.

Contents

1. Introduction

This compilation provides heat capacity and entropy data on approximately 1300 organic compounds in the liquid and solid phases. Data on the enthalpies and entropies of phase transitions which have been determined from calorimetric measurements are also included. A total of 565 articles have been examined, evaluated, and referenced.

This compilation is a supplement to an earlier document published in 1984, namely, "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase" by E. S. Domalski, W. H. Evans, and E. D. Hearing, J. Phys. Chem. Ref. Data, **13**, Suppl. 1, (1984). Since 1984, two large compilations have been published which contain data on the thermodynamic properties of organic compounds in the condensed phase; they are:

"Thermodynamic Properties of Oxygen-Containing Organic Compounds", by I. A. Vasil'ev and V. M. Petrov, Handbook, Leningrad, 240 pages (1984).

"Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 1. Properties of Condensed Phases by R. C. Wilhoit, J. Chao, and K. R. Hall, J. Phys. Chem. Ref. Data, **14**, 1 (1985).

The latter two compilations were useful in assisting us with the completeness of our search of the literature for papers on heat capacities, entropies, and phase transition properties of organic oxygen compounds. The discus-

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sions on specific compounds provided by Wilhoit, Chao, and Hall were helpful in the assignment of a rating to our evaluation of those data.

2. Scope of the Search

References containing data on the heat capacities and entropies of organic compounds in the condensed phase were obtained through a search of the files of the Chemical Thermodynamics Data Center of the National Institute of Standards and Technology. Additional references were located through the Bulletin of Chemical Thermodynamics and through Chemical Abstracts. The original papers were examined to obtain the data which has been tabulated, to determine whether corrections should be applied, and to qualitatively evaluate the reported measurements.

Our previous publication [1], covered the literature from 1881 to the beginning of 1982. About half of the 565 papers referenced in this publication contain measurements performed for that same period of time with the remaining half covering the period from 1982 to most of 1989.

The goal of the search has been to obtain heat capacity and entropy data for organic compounds at "room temperature", however, the temperature range included is 200–450 K. This extended range was chosen so that the user would have, whenever possible, values for temperatures close to room temperature even if the measurement range did not include 298.15 K. Usually, the user can extrapolate such data to 298.15 K or to temperatures outside of the reported range if desired.

Values of the enthalpy and entropy of phase transitions — solid/solid, solid/liquid, as well as some solid/gas, and liquid/gas transitions — obtained from calorimetric measurements are included along with the data on heat capacity and entropy. No specific search was made for the transition properties. They are included as a by-product of the search for experimental heat capacity data.

Corrections for relative atomic mass (atomic weight), temperature scale, and energy units have been made, where appropriate. Values have been reported at "298 K" with the ice point taken as 273.1, 273.15, or 273.16 K; the correction for this small change is much less than the precision and accuracy of the data. Some researchers did not provide tabulated values of C_p and S as a function of temperature, but gave an equation, such as: $C_p = A + BT + CT^2$. In these cases, a value for C_p and/or S at 298 K was derived from the equation provided. Some researchers have provided only graphs of C_p as a function of temperature. For good quality graphs, estimates of C_p at 298 K were extracted and correspondingly identified. Care was taken to assure that heat capacity data reported in International Steam Table (IT) energy units were converted to the International System of Units (SI Units). Except for very precise data, corrections involving energy units for most measurements since about 1930 are often within the uncertainty of the data. Older data are of lower precision so that corrections are not needed. In general, transition temperatures are those reported by the investigator. The effort to convert each investigator's temperature scale to the 1968 International Practical Temperature Scale (IPTS-68) was not warranted. Hence, the reported values may have a systematic error of up to 0.1 K. Fortunately, modern high-precision measurements are usually based on IPTS-68.

3. Arrangement of the Data

The table of heat capacities, entropies, and phase transitions given in this paper contains data entries for a variety of organic compounds. The entries here, as in the 1984 J. Phys. Chem. Ref. Data publication [1], are arranged in the order of the empirical formulae of the compounds; isomers are further separated by their Wiswesser Line Notation [2]. The latter notation system has been used to represent the structure of the organic compound. Under a given organic substance, the data from the pertinent papers are included. The data from each paper form a separate entry, complete with identification of the reference source. When there are several reference entries for a compound, they are arranged chronologically by year.

For each entry the data given are: molecular (empirical) formula for the compound, physical state, reference code, compound name(s), followed by the values for the heat capacity, entropy, and, where available, phase transition data. The entry of information is completed by the molecular weight, Wiswesser Line Notation for the compound, and a graduated indication of the quality of the data. The formula given is the empirical formula for the compound; water of hydration is shown as $\cdot(n)H_2O$. The elements are arranged in the order C, H(D, T), followed by the other elements in alphabetical order of their chemical symbols. One or more names are given for each compound. No attempt has been made to conform to a rigorously systematic nomenclature. Common names and systematic names are used; alternate names have been given freely. All names used appear in the Compound Name-Formula Index in Sec. 8, which should assist the reader who is aware of the compound name but not its empirical formula.

The bibliography is listed in Sec. 9. The reference code is of the form XXAAA/BBBN where XX are the last two digits of the year of publication of the paper, AAA is the first three letters of the last name of the first author and BBB is the first three letters of the last name of the second author (if present). Authors after the first two are disregarded. N is a digit from 2 to 9 used to indicate a second, third, ...paper with the same year and author codes. Thus, 60BRO/SMI2 refers to a paper by Brown and Smith appearing in 1960, the second one with authors BRO... and SMI...; 44JON is a 1944 paper by Jones. The full citation appears in the bibliography

arranged according to the reference codes. For papers published before 1900, all four digits for the year are used.

When authors have given a table of smoothed values for the heat capacity, the value at 298 K (interpolated if necessary) or the value nearest to that temperature is given. If experimental measurements are represented only by a smoothing equation, this is used to calculate the value given. If only the unsmoothed experimental results are given by the authors, one of these is given, with the corresponding temperature. Such a selection is accompanied by a remark.

The third-law entropy is given at 298 K or at the temperature closest to this temperature. The value is that obtained by the authors; we have not reintegrated the heat capacity data to re-evaluate the entropy.

Phases are indicated by g, liq, c, c,I, c,II, etc. In general, no attempt has been made to specify the crystalline form of the solid phases; c,I is used for the form stable at the melting point. For each phase transition, the appropriate process, i.e., c/liq, the temperature in kelvins, the enthalpy and entropy change for the isothermal process, and when appropriate, the pressure, are given. The entropy change ΔS is taken as $\Delta H/T$ unless indicated otherwise. Energy values are given in joules and can be related to the thermochemical calorie by the conversion factor: 4.1840 joules equals one thermochemical calorie. Pressures are given in kilopascals; one standard atmosphere is 101.325 kPa.

The molecular weight is based upon the 1987 IUPAC Table of International Atomic Weights [3]. Two exceptions are made; the atomic weights of hydrogen, nitrogen, and fluorine are taken as 1.0079, 14.0067, and 18.9984 rather than 1.00794, 14.00674, and 18.9984032, respectively. When the molecular weight differs from that originally used by the authors, appropriate corrections to the values have been made.

An indication of our general evaluation of the data reported is given as A (high quality), B (good), C (average), and D (low quality). This rating is based upon the method used, the details of the measurements as reported, the number of measurements, purity of the sample, calibrations, and corrections applied to the data; it is intended as a guide to those data we feel are more reliable. In addition, the number of significant figures given for the numerical values indicates roughly the quality of the data. In general, papers that are rated as being of high quality provide a detailed description of the cryostat used, the experimental procedure, the purity and characterization of the sample, calibration results, both raw and smoothed data for the temperature range over which measurements were made, and comment on the precision and accuracy of their data. An absence of numerical or descriptive information, or poor agreement with a detailed and accurate study can lead to a low rating.

All of the names used to identify the compounds are included in the Compound Name-Formula Index with the appropriate empirical fomulae. Prefixes such as *tert-*, *ortho-*, α-, 1,2-, (but not *Iso*) are disregarded in the alphabetization of the names.

The sequencing of the compounds is based on the empirical formula. The formulae are sorted alphabetically by the first atomic symbol, then by the number of atoms of this element present (the Hill Indexing System [4]). As was the practice with the 1984 J. Phys. and Chem. Ref. Data publication [1], C, carbon, is always the first element. This arranged list of formulae is then sorted by the second atomic symbol (H, hydrogen, if present), and then by the number of atoms of this element. The sorting proceeds alphabetically thereafter for each element present. The following list illustrates this scheme:

C
CCl_4
$CHCl_3$
CH_4
CO_2
$C_2Cl_3O_2$
$C_2H_2Cl_2$
C_2H_3Cl
C_2H_4
$C_2H_4O_2$
C_2H_6
C_2H_6O

Isomeric compounds are further sorted by their Wiswesser Line Notation:

$C_4H_{10}O$	2O2	$C_2H_5OC_2H_5$
	3O1	$C_3H_7OCH_3$
	Q1Y1&1	$(CH_3)_2CHCH_2OH$
	QX1&1&1	$(CH_3)_3COH$
	QY2&1	$C_2H_5CH(CH_3)OH$

4. Definitions

Heat Capacity. The heat capacity is defined as the derivative of the energy of the system with respect to the temperature under specified conditions. The heat capacity may be stated as an average value over a temperature range or the limiting value over an infinitesmal temperature change. If the system is maintained at constant volume, the heat capacity, C_v, is given by the derivative of energy with respect to temperature,

$$C_v = (\partial U/\partial T)_v$$

where U is the internal energy.

If the system is maintained at constant pressure, the heat capacity, C_p, is given by:

$$C_p = (\partial H/\partial T)_P$$

where H is the enthalpy.

The values of heat capacity reported in this paper are those at constant pressure and correspond to one mole of a specified substance; the units are thus, $J \cdot mol^{-1} \cdot K^{-1}$.

Experimentally, the heat capacity, C_p, is obtained from the enthalpy change at constant pressure over a small temperature change. This value is associated with the temperature at the midpoint of the temperature range:

$$C_p = \Delta H/(T_2 - T_1) \text{ at } (T_1 + T_2)/2.$$

Actual heat capacity measurements, or C_{sat}, for liquids and solids are normally made with the sample in equilibrium with its own vapor or saturation pressure; the correction from C_{sat} to C_p at the standard pressure, 101.325 kPa (1 atm) is usually negligible for solids and for liquids below their boiling point. For volatile organic compounds in the condensed phase, a correction for the enthalpy of vaporization of the condensed phase as well as the heat capacity of the vapor phase must be applied.

For nonvolatile solid organic compounds, the relationship between C_p and C_{sat} is given by:

$$C_p - C_{sat} = [T(\partial P/\partial T)_{sat}][(\partial V/\partial T)_P]$$

where $(\partial P/\partial T)_{sat}$ is the slope of the vapor or saturation pressure curve and $(\partial V/\partial T)_P$ is the volume expansivity of the solid. Again, the magnitude of this correction is usually negligible.

Entropy. For totally reversible processes, the entropy change of a system is equal to the amount of heat, Q, absorbed by the system divided by the temperature, T. For an infinitesmal change in entropy:

$$dS = dQ/T \ .$$

Entropy and heat capacity are related by the following expressions:

$(\partial S/\partial T)_v = C_v/T$, at constant volume,
$(\partial S/\partial T)_p = C_p/T$, at constant pressure,
$(\partial S/\partial T) = C_{sat}/T$, at equilibrium vapor pressure along the two phase line.

The (calorimetric) entropy is obtained by integration of the measured values of C_p/T from the lowest temperature of measurement to the reported temperature. Various methods have been used to extrapolate from the lowest experimental temperature to zero kelvin. Appropriate values of the entropies of phase changes must be added. The entropy at zero kelvin is taken as zero for the stable crystalline state, with the addition of residual (zero point) entropy, not removed by the extrapolation, due to non-random ordering, optical isomerism, or multiple electronic ground states for the molecule. Thus,

$$S_T^\circ = S_0^\circ(\text{zero point}) + \int_0^{T_1} (C_p/T)dT \,(\text{extrapolation}) +$$
$$\int_{T_1}^{T_2} (C_p/T)dT + \Delta H_{T_2}/T_2 \,(\text{phase change}) +$$
$$\int_{T_2}^{T_3} (C_p/T)dT + \Delta H_{T_3}/T_3 \,(\text{phase change}) +$$
$$\int_{T_3}^{T} (C_p/T)dT$$

For additional discussions on the concept of entropy, the reader should consult references [5] and [6].

Phase Transitions. A process by which a substance undergoes a change of physical state, i.e., solid-solid, solid-liquid, solid-gas, or liquid-gas, is known as a phase transition or phase change. The phase change is accompanied by a transfer of energy (commonly referred to as latent heat) and a change in volume while both temperature and pressure remain constant. For a phase change which is carried out reversibly (i.e., under equilibrium conditions) at a constant temperature and pressure, the total Gibbs energy remains unchanged. If there is an enthalpy (or heat) change, then it follows that there will also be an entropy change for the process, because:

$$\Delta H - \Delta ST = 0, \text{ or } \Delta S = \Delta H/T \ .$$

These equations are applicable only for the temperature and pressure at which the phases are in equilibrium.

For phase changes — solid-solid, solid-liquid, solid-gas, liquid-gas — encountered in the accompanying tables in Sec. 7, ΔH refers to the isothermal enthalpy change at the transition temperature. Corrections can be applied to the experimental data for premelting effects to isothermal conditions. The pressure, unless specified, is the vapor pressure of the substance at the transition temperature; the correction to a standard state pressure is usually negligible at ordinary pressures for a solid-solid transition and for fusion. The entropy change is taken as $\Delta H/T$ at the equilibrium pressure.

Some investigators have reported the measurement of anomalous phase changes in which the volume and entropy are continuous, but the heat capacity is discontinuous. During such phase changes no latent heat is present and the shape of the curve of the heat capacity plotted as a function of temperature often resembles the Greek letter lambda at the transition point. Such a transition is called a "lambda transition". In order to differentiate these anomalous transitions from ordinary phase changes, it has become customary to identify normal phase changes as phase changes of the first order and atypical phase changes as those of the second order. The discontinuity which occurs in a first order phase transition is a commonly observed phenomenon; however, the discontinuity associated with a second order phase transition has been more difficult to identify and/or interpret. Sometimes the discontinuous nature of the heat capacity is questioned in a second order transition because experimental measurements show a peak or a hump at the transition temperature rather than an unambiguous discontinuity.

A phase change which is accompanied by changes in the entropy and volume and whose first-order derivatives of the Gibbs energy with respect to temperature and pressure change discontinuously is known as a phase change of the first order,

$$S = -(\partial G/\partial T)_P, \text{ and } V = (\partial G/\partial P)_T.$$

A phase change which is accompanied by changes in the heat capacity, volume expansivity, and isothermal compressibility and whose second order derivatives of the Gibbs energy with respect to temperature and pressure change discontinuously is known as a phase change of the second order,

$$C_p/T = (\partial S/\partial T)_P = -(\partial^2 G/\partial T^2)_P$$

$$KV = -(\partial V/\partial P)_T = -(\partial^2 G/\partial P^2)_T$$

$$\beta V = (\partial V/\partial T)_P = (\partial^2 G/\partial T \partial P)_{T,P},$$

where K is the isothermal compressibility and β is the volume expansivity. The relationship between these quantities and the pressure and temperature is given below by Ehrenfest's eq. [7].

$$dP/dT = [C_p(f) - C_p(i)]/[TV(\beta(f) - \beta i))],$$

$$dP/dT = [\beta(f) - \beta(i)]/[K(f) - K(i)],$$

where i and f represent the initial and final states of the phase change.

For additional discussion regarding first and second order phase transitions, the reader should consult references [8, 9, and 10].

5. Acknowledgements

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6. References for the Introductory Discussion

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7. Table of Heat Capacities, Entropies, and Phase Transition Properties

C (c) 73BUT/MAD
Graphite; Carbon, graphite
Heat Capacity 300 K, $C_p = 8.6186$ J·mol^{-1}·K^{-1}
Temperature range 200 to 3500 K.
Least squares fit of 'best' data gives: $C_p = 0.538657 + 9.11129\times10^{-6}T - 90.2725T^{-1} - 43449.3T^{-2} + 1.59309\times10^{7}T^{3} - 1.43688\times10^{9}T^{-4}$ cal·g^{-1}·K^{-1} (250 to 3000 K).
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A
Results from an evaluation of literature data.

C (c) 73MAR/VOL
Graphite; Carbon, graphite, single-crystal
Heat Capacity 298.15 K, $C_p = 8.11$ J·mol^{-1}·K^{-1}
Temperature range 1 to 3000 K. $C_p = 0.6752$ J·g^{-1}·K^{-1}.
Entropy 298.15 K, $S = 5.51$ J·mol^{-1}·K^{-1}
$S^{\circ}_T = 0.4585$ J·g^{-1}·K^{-1}.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A
Results from an evaluation of literature data.

C (c) 76VOL/BUC
Diamond; Carbon, diamond
Heat Capacity 300 K, $C_p = 6.57$ J·mol^{-1}·K^{-1}
Temperature range 300 to 1200 K.
Natural diamond;
C_p calculated by extrapolation of value at 350 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation C

C (c) 76VOL/BUC
Diamond; Carbon, diamond
Heat Capacity 300 K, $C_p = 6.61$ J·mol^{-1}·K^{-1}
Temperature range 75 to 1200 K.
SAM synthetic diamond.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation C

C (c) 76VOL/BUC
Diamond; Carbon, diamond
Heat Capacity 300 K, $C_p = 6.37$ J·mol^{-1}·K^{-1}
Temperature range 75 to 1200 K.
Ballas synthetic diamond.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation C

C (c) 81ISA/WAN
Graphite; Carbon, graphite
Heat Capacity 300 K, $C_p = 10.05$ J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
$C_p = 8.729\times10^{-4}T + 6.27\times10^{-6}T^{2} + 6.309\times10^{-9}T^{3}$ J·g^{-1}·K^{-1}.
Value calculated from equation.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation B
Poco process graphite AXM-5Q1.

C (c) 87DOB/PER
Carbon; Graphite
Heat Capacity 350 K, $C_p = 10.68$ J·mol^{-1}·K^{-1}
Temperature range 300 to 1800 K.
Molecular Weight 12.0110
Wiswesser Line Notation C
Evaluation A
POCO AXM-5Q1 graphite.

CBr_4 (c) 84BIC/MIN
Carbon tetrabromide; Tetrabromomethane
Heat Capacity 298.15 K, $C_p = 145.9$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.44 J·K^{-1}·g^{-1}.
Molecular Weight 331.6270
Wiswesser Line Notation EXEEE
Evaluation B

CCl_3F (liq) 82MAR
Fluorotrichloromethane; Freon 11
Phase Changes
c/liq 165.4 K, $\Delta H = 7900$ J·mol^{-1}
$\Delta S = 47.8$ J·mol^{-1}·K^{-1}
Molecular Weight 137.3684
Wiswesser Line Notation GXFGG
Evaluation C

CCl_4 (liq) 57HAR/MOE
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 303.3 K, $C_p = 130.5$ J·mol^{-1}·K^{-1}
Temperature range 254 to 303 K.
Unsmoothed experimental datum.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation C

CCl_4 (liq) 76FOR/BEN2
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, $C_p = 131.401$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 76MOR/RIC
Carbon tetrachloride; Tetrachloromethane
Phase Changes
c,II/c,I 225.7 K, $\Delta H = 4631$ J·mol^{-1}
$\Delta S = 20.52$ J·mol^{-1}·K^{-1}
(c,II/c,Ib)
c,I/liq 250.53 K, $\Delta H = 2562$ J·mol^{-1}
$\Delta S = 10.226$ J·mol^{-1}·K^{-1}
(c,Ib/liq). Data also given for (c,Ia/liq):
246.00 K, $\Delta H = 1830$ J·mol^{-1}.
$\Delta S = 7.44$ J·mol^{-1}·K^{-1}
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation A

CCl_4 (liq) 77VES/SVO
Carbon tetrachloride; Tetrachloromethane
Heat Capacity 298.15 K, $C_p = 131.40$ J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 153.8230
Wiswesser Line Notation GXGGG
Evaluation B

CF_3Br (liq) 84STO/CHA
Bromotrifluoromethane
Heat Capacity 293 K, C_p = 163.8 J·mol^{-1}·K^{-1}
Temperature range 163 to 293 K.
Molecular Weight 148.9102
Wiswesser Line Notation FXEFF
Evaluation C

CF_4 (liq) 69ENO/SHI
Carbon tetrafluoride; Tetrafluoromethane; Freon 14
Heat Capacity
Temperature range 4 to 100 K.
Phase Changes
c,II/c,I 76.09 K, ΔH = 1462.3 J·mol^{-1}
ΔS = 19.20 J·mol^{-1}·K^{-1}
c,I/liq 89.529 K, ΔH = 705.4 J·mol^{-1}
ΔS = 7.87 J·mol^{-1}·K^{-1}
Molecular Weight 88.0046
Wiswesser Line Notation FXFFF
Evaluation A

$(CH)_n$ (c) 83LEI/KAH
Polyacetylene
Heat Capacity 300 K, C_p = 60 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K. Cis isomer.
C_p = 40 J·mol^{-1}·K^{-1} for trans isomer.
Data given graphically. Data estimated from graph.
Molecular Weight 13.0189
Wiswesser Line Notation /*YUY*/
Evaluation D

$CHBr_3$ (liq) 84GOL/KOL
Tribromomethane; Bromoform
Phase Changes
c/liq 281.84 K, ΔH = 11046 J·mol^{-1}
ΔS = 39.2 J·mol^{-1}·K^{-1}
Molecular Weight 252.7309
Wiswesser Line Notation EYEE
Evaluation A

$CHCl_3$ (liq) 57HAR/MOE
Trichloromethane; Chloroform
Heat Capacity 303.2 K, C_p = 114.0 J·mol^{-1}·K^{-1}
Temperature range 245 to 303 K.
Unsmoothed experimental datum.
Molecular Weight 119.3779
Wiswesser Line Notation GYGG
Evaluation C

$CHNaO_2$ (c) 83FRA/PLA
Sodium methanoate; Sodium formate
Heat Capacity 298.15 K, C_p = 87.68 J·mol^{-1}·K^{-1}
Temperature range 300 to 520 K.
C_p data taken from 60WES/CHA in temperature range 5 to 350 K.
Entropy 298.15 K, S = 103.76 J·mol^{-1}·K^{-1}
S data taken from 60WES/CHA.
Phase Changes
c,II/c,I 491.5 K, ΔH = 1214 J·mol^{-1}
ΔS = 2.47 J·mol^{-1}·K^{-1}
c,I/liq 530.46 K, ΔH = 17710 J·mol^{-1}
ΔS = 33.39 J·mol^{-1}·K^{-1}
Molecular Weight 68.0075
Wiswesser Line Notation VHO .NA
Evaluation A

CHO_2Tl (c) 76MEI/SEY
Thallium formate
Phase Changes
c,I/liq 374 K, ΔH = 10878 J·mol^{-1}
ΔS = 28.9 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 249.3877
Wiswesser Line Notation VHO .TL
Evaluation B

$(CH_2)_n$ (c) 57SOC/TRA
Polyethylene
Heat Capacity 270 K, C_p = 24.4 J·mol^{-1}·K^{-1}
Temperature Range 58 to 270 K.
C_p value is unsmoothed experimental datum.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation B

$(CH_2)_n$ (c) 61WAR/PET
Polyethylene
Heat Capacity 300 K, C_p = 31.69 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K. Interpolated data.
Entropy 300 K, S = 25.52 J·mol^{-1}·K^{-1}
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A
Branched, high pressure polyethylene.

$(CH_2)_n$ (c) 62WUN
Polyethylene
Heat Capacity 300 K, C_p = 24.53 J·mol^{-1}·K^{-1}
Temperature range 1 to 420 K.
Extrapolated value to 100% crystalline phase.
Entropy 300 K, S = 24.04 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 415 K, ΔH = 3879 J·mol^{-1}
ΔS = 9.35 J·mol^{-1}·K^{-1}
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (amorph) 62WUN
Polyethylene
Heat Capacity 300 K, C_p = 32.85 J·mol^{-1}·K^{-1}
Temperature range 1 to 420 K.
Extrapolated value to 100% amorphous phase.
Entropy 300 K, S = 31.96 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 415 K, ΔH = 3879 J·mol^{-1}
ΔS = 9.35 J·mol^{-1}·K^{-1}
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation A

$(CH_2)_n$ (c) 78STE
Polyethylene
Heat Capacity 298.15 K, C_p = 25.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 14.0268
Wiswesser Line Notation /*1*/
Evaluation B

CH_2Cl_2 (liq) 57HAR/MOE
Dichloromethane; Methylene dichloride
Heat Capacity 303.2 K, $C_p = 105.5$ J·mol^{-1}·K^{-1}
Temperature range 244 to 303 K.
Unsmoothed experimental datum.
Molecular Weight 84.9328
Wiswesser Line Notation G1G
Evaluation C

CH_2N_2 (c) 83DEW/DEK
Cyanamid
Heat Capacity 300 K, $C_p = 78.2$ J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Linearly extrapolated.
Phase Changes
c/liq 318.71 K, $\Delta H = 7272$ J·mol^{-1}
$\Delta S = 22.82$ J·mol^{-1}·K^{-1}
Molecular Weight 42.0402
Wiswesser Line Notation ZCN
Evaluation B(C_p), A(Phase changes).

CH_3Cl_3Si (liq) 71SAM/KOS2
Trichloromethylsilane
Heat Capacity 298.15 K, $C_p = 163.1$ J·mol^{-1}·K^{-1}
Temperature range 14 to 307 K.
Data deposited VINITI, No 2423-71, 17 December, 1970.
C_p(liq) = 25.5286 + 0.04132T + 100930T^{-2}
(197.37 to 300 K) cal·mol^{-1}·K^{-1}.
Entropy 298.15 K, $S = 262.8$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 197.37 K, $\Delta H = 8945$ J·mol^{-1}
$\Delta S = 45.31$ J·mol^{-1}·K^{-1}
Molecular Weight 149.4792
Wiswesser Line Notation G-SI-GG1
Evaluation A
Debye temperature = 98.84 K.

CH_3NO (liq) 76SKO/SUU
Formamide; Methanamide
Heat Capacity 298.15 K, $C_p = 107.62$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation A

CH_3NO (liq) 83DEW/DEK
Formamide; Methanamide
Heat Capacity 298.15 K, $C_p = 107.61$ J·mol^{-1}·K^{-1}
Temperature range 90 to 290 K.
C_p = 89.88 + 0.05947 (T/K) J·mol^{-1}·K^{-1} (275 to 300 K).
Phase Changes
c/liq 275.60 K, $\Delta H = 8667$ J·mol^{-1}
$\Delta S = 31.448$ J·mol^{-1}·K^{-1}
Molecular Weight 45.0408
Wiswesser Line Notation ZVH
Evaluation A

CH_4 (c) 76VOG/PIT
Methane
Heat Capacity
Temperature range 0.4 to 28 K.
Phase Changes
c,II/c,I 20.53 K, $\Delta H = 93.55$ J·mol^{-1}
$\Delta S = 4.557$ J·mol^{-1}·K^{-1}
Lambda transition.
c,I/liq 90.67 K, $\Delta H = 939.2$ J·mol^{-1}
$\Delta S = 10.36$ J·mol^{-1}·K^{-1}
liq/g 99.54 K, $\Delta H = 8519$ J·mol^{-1}
$\Delta S = 85.58$ J·mol^{-1}·K^{-1}
$p = 32.81$ kPa
Data from 37FRA/CLU and 39FRA/CLU.
Molecular Weight 16.0426
Wiswesser Line Notation 1H
Evaluation A

CH_4N_2O (c) 03MAG
Urea
Heat Capacity 298 K, $C_p = 80.7$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.321 cal·g^{-1}·K^{-1}.
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation D

CH_4N_2O (c) 80VOG/SCH
Urea
Heat Capacity
Temperature range 323 to 493 K. Equation only:
$C_p = 523.38 - 265.60\times10^{-2}T + 41.50\times10^{-4}T^2$.
Phase Changes
c/liq 405.8 K, $\Delta H = 13610$ J·mol^{-1}
$\Delta S = 33.54$ J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation B
Dry sample.

CH_4N_2O (c) 86KOZ/DAL
Urea
Heat Capacity 298.15 K, $C_p = 93.08$ J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K. $C_p = 38.43 + 4.98\times10^{-2}T + 7.05\times10^{-4}T^2 - 8.61\times10^{-7}T^3$ (240 to 400 K).
Entropy 298.15 K, $S = 104.93$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 405.8 K, $\Delta H = 13900$ J·mol^{-1}
$\Delta S = 34.25$ J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

CH_4N_2O (c) 87DEL/FER
Urea
Phase Changes
c/liq 406.5 K, $\Delta H = 14790$ J·mol^{-1}
$\Delta S = 36.4$ J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation A

CH_4N_2O (c) 88GAM/BRO
Urea
Heat Capacity 304.7 K, $C_p = 94.0$ J·mol^{-1}·K^{-1}
Temperature range 303 to 413 K.
Phase Changes
c/liq 406 K, $\Delta H = 14500$ J·mol^{-1}
$\Delta S = 35.7$ J·mol^{-1}·K^{-1}
Molecular Weight 60.0554
Wiswesser Line Notation ZVZ
Evaluation B

CH_4N_2S (c) 67WES/CHA
Thiourea
Heat Capacity 298.15 K, $C_p = 96.90$ J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K
Entropy 298.15 K, $S = 115.8$ J·mol^{-1}·K^{-1}
Molecular Weight 76.1160
Wiswesser Line Notation ZYZUS
Evaluation A
Anomalies occur at: 169.3 K, $\Delta S = 0.17$ J·mol^{-1}·K^{-1}; 171.2 K, $\Delta S = 0.04$ J·mol^{-1}·K^{-1}; 200 K, $\Delta S = 0.71$ J·mol^{-1}·K^{-1}. A slight hump in the heat capacity appears between 210 and 260K.

CH_4N_2S (c) 82TOR/SAB
Thiourea
Heat Capacity 298.15 K, $C_p = 96.90$ J·mol^{-1}·K^{-1}
One temperature. C_p data given as 1.273 J·K^{-1}·g^{-1}.
Data from 67WES/CHA.
Phase Changes
c/g 298.15 K, $\Delta H = 112000$ J·mol^{-1}
$\Delta S = 375.6$ J·mol^{-1}·K^{-1}
Molecular Weight 76.1160
Wiswesser Line Notation ZYZUS
Evaluation B

CH_4O (liq) 82VIL/CAS
Methanol; Methyl alcohol
Heat Capacity 298.15 K, $C_p = 81.92$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 84ZEG/SOM
Methanol; Methyl alcohol
Heat Capacity 298.15 K, $C_p = 81.47$ J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 86KOR/KUK
Methanol; Methyl alcohol
Heat Capacity 298 K, $C_p = 81.32$ J·mol^{-1}·K^{-1}
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (liq) 86TAN/TOY
Methanol; Methyl alcohol
Heat Capacity 298.15 K, $C_p = 81.56$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

CH_4O (liq) 88OKA/OGA
Methanol; Methyl alcohol
Heat Capacity 298.15 K, $C_p = 80.35$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation B

CH_4O (gls) 68SUG/SUG
Methanol; Methyl alcohol
Heat Capacity 120 K, $C_p = 68.39$ J·mol^{-1}·K^{-1}
Temperature range 20 to 120 K.
Phase Changes
c/gls 103 K, $\Delta H = 1540$ J·mol^{-1}
$\Delta S = 14.95$ J·mol^{-1}·K^{-1}
Glass transition.
c/liq 175.22 K
Molecular Weight 32.0420
Wiswesser Line Notation Q1
Evaluation A

$CH_4N_2S \cdot HNO_3$ (c) 84NUR/BER
Thiourea nitrate
Heat Capacity 298.15 K, $C_p = 175.4$ J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, $S = 213.5$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 265.3 K, $\Delta H = 34.0$ J·mol^{-1}
$\Delta S = 0.130$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1288
Wiswesser Line Notation ZYZUS &WNQ
Evaluation A

CH_5N_3O (c) 86LEB/KUL
Semicarbazide
Heat Capacity 298.15 K, $C_p = 110.6$ J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, $S = 119.6$ J·mol^{-1}·K^{-1}
Molecular Weight 75.0700
Wiswesser Line Notation ZVMZ
Evaluation A

CH_5N_3S (c) 82TOR/SAB
Thiosemicarbazide
Heat Capacity 298.15 K, $C_p = 110.9$ J·mol^{-1}·K^{-1}
One temperature. C_p data given as 1.217 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, $\Delta H = 125800$ J·mol^{-1}
$\Delta S = 421.9$ J·mol^{-1}·K^{-1}
Molecular Weight 91.1306
Wiswesser Line Notation ZYMZUS
Evaluation B

CH_5N_3S (c) 84NUR/BER
Thiosemicarbazide
Heat Capacity 298.15 K, $C_p = 114.3$ J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, $S = 128.2$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 268.9 K, $\Delta H = 70.0$ J·mol^{-1}
$\Delta S = 0.250$ J·mol^{-1}·K^{-1}
Molecular Weight 91.1306
Wiswesser Line Notation ZYMZUS
Evaluation A

CH_6IN (c) 86YAM/OGU
Methylammonium iodide
Heat Capacity 298.15 K, C_p = 93.93 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S = 160.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 166.1 K
Undercooled α' to metastable δ.
Molecular Weight 158.9696
Wiswesser Line Notation Z1 &IH
Evaluation A
Data given for β' phase from 10 to 220 K.
β' to α' phase transition at 220 K,
ΔH = 2970 J·mol^{-1}, ΔS = 13.5 J·mol^{-1}·K^{-1}.

CH_6N_4S (c) 82TOR/SAB
Thiocarbohydrazide
Heat Capacity 298.15 K, C_p = 125.3 J·mol^{-1}·K^{-1}
One temperature. C_p data given as 1.180 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, ΔH = 152100 J·mol^{-1}
ΔS = 510.1 J·mol^{-1}·K^{-1}
Molecular Weight 106.1452
Wiswesser Line Notation ZMYMZUS
Evaluation B

$C_2Br_2F_4$ (liq) 88VES/ZAB
1,2-Dibromotetrafluoroethane
Heat Capacity 298.15 K, C_p = 173.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
C_p(J·mol^{-1}·K^{-1}) = 131.53 + 0.1420(T/K) (298 to 318 K).
Molecular Weight 259.8236
Wiswesser Line Notation FXFEXFFE
Evaluation A

$C_2CaO_4.H_2O$ (c) 33LAT/SCH
Calcium oxalate monohydrate
Heat Capacity 299.78 K, C_p = 152.4 J·mol^{-1}·K^{-1}
Temperature Range 19 to 300 K;
C_p value is unsmoothed experimental datum.
Entropy 298.1 K, S = 156.0 J·mol^{-1}·K^{-1}
Molecular Weight 146.1128
Wiswesser Line Notation OVVO.CA &QH
Evaluation B

C_2ClF_3 (liq) 84GOL/KOL
Chlorotrifluoroethene; Chlorotrifluoroethylene;
Trichlorofluoroethene; Trichlorofluoroethylene
Phase Changes
c/liq 118.3 K, ΔH = 5282 J·mol^{-1}
ΔS = 44.6 J·mol^{-1}·K^{-1}
Molecular Weight 116.4702
Wiswesser Line Notation GYFUYFF
Evaluation A

$C_2Cl_3F_3$ (liq) 84GOL/KOL
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Phase Changes
c/liq 273.93 K, ΔH = 2326 J·mol^{-1}
ΔS = 8.49 J·mol^{-1}·K^{-1}
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation A

$C_2Cl_3F_3$ (liq) 88VES/ZAB
1,1,2-Trichloro-1,2,2-trifluoroethane; Freon 113
Heat Capacity 298.15 K, C_p = 172.9 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
C_p(J·mol^{-1}·K^{-1}) = 113.21 + 0.1991(T/K) (240 to 337 K).
Molecular Weight 187.3762
Wiswesser Line Notation GXGFXGFF
Evaluation A

$C_2Cl_3F_3$ (liq) 87OTT/WOO
1,1,1-Trichlorotrifluoroethane
Phase Changes
c,II/c,I 148 K
Solid-plastic crystal.
c,I/liq 287.52 K, ΔH = 4110 J·mol^{-1}
ΔS = 14 J·mol^{-1}·K^{-1}
Molecular Weight 187.3762
Wiswesser Line Notation GXGGXFFF
Evaluation A

$C_2Cl_3F_3$ (liq) 88SVO/VES
1,1,1-Trichlorotrifluoroethane
Heat Capacity 298.16 K, C_p = 168.6 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
C_p(J·mol^{-1}·K^{-1}) = 109.0 + 0.200 (T/K) (298 to 318 K).
Molecular Weight 187.3762
Wiswesser Line Notation GXGGXFFF
Evaluation A

C_2Cl_4 (liq) 86NOV/RAB
Tetrachloroethylene; Tetrachloroethene
Heat Capacity 298.15 K, C_p = 157.9 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 298.15 K, S = 240.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 125–210 K, ΔH = 820 J·mol^{-1}
ΔS = 5.26 J·mol^{-1}·K^{-1}
c/liq 250.81 K, ΔH = 10880 J·mol^{-1}
ΔS = 43.38 J·mol^{-1}·K^{-1}
Molecular Weight 165.8340
Wiswesser Line Notation GYGUYGG
Evaluation A

$C_2Cl_4F_2$ (c) 84GOL/KOL
1,1,1,2-Tetrachlorodifluoroethane
Phase Changes
c/liq 314.2 K, ΔH = 3990 J·mol^{-1}
ΔS = 12.7 J·mol^{-1}·K^{-1}
Molecular Weight 203.8308
Wiswesser Line Notation GXGGXGFF
Evaluation *A*

C_2Cl_6 (c) 50SEK/MOM
Hexachloroethane
Heat Capacity 298.5 K, C_p = 218.0 J·mol^{-1}·K^{-1}
Temperature range 295 to 351 K.
Unsmoothed experimental datum.
Phase Changes
c,III/c,II 318 K, ΔH = 2565 J·mol^{-1}
ΔS = 8.08 J·mol^{-1}·K^{-1}
c,II/c,I 345 K, ΔH = 8222 J·mol^{-1}
ΔS = 23.8 J·mol^{-1}·K^{-1}
c,I/liq 458 K, ΔH = 9749 J·mol^{-1}
ΔS = 23.0 J·mol^{-1}·K^{-1}
Molecular Weight 236.7400
Wiswesser Line Notation GXGGXGGG
Evaluation B(C_p), A(Phase changes)

$C_2D_{12}C_{16}N_2Sn$ (c) 88MAT/YAN
Bis(methylammonium-d_6) hexachlorostannate (IV)
Heat Capacity 298.15 K, C_p = 321.68 J·mol^{-1}·K^{-1}
Temperature Range 13 to 300 K
Entropy 298.15 K, S = 498.62 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 154.96 K, ΔH = 2810 J·mol^{-1}
ΔS = 21.8 J·mol^{-1}·K^{-1}
Order/disorder transition
Molecular Weight 407.6512
Wiswesser Line Notation 1ZH 2 -SN- G6 &1/H-2 3 &2/H-2 3
Evaluation A

$C_2F_2O_2$ (liq) 71HOD
Oxalyl fluoride
Heat Capacity
Temperature range 13 to 270 K.
Phase Changes
c/liq 260.73 K, ΔH = 13407 J·mol^{-1}
ΔS = 51.4 J·mol^{-1}·K^{-1}
liq/g 270.13 K, ΔH = 28255 J·mol^{-1}
ΔS = 104.6 J·mol^{-1}·K^{-1}
Molecular Weight 94.0176
Wiswesser Line Notation FVVF
Evaluation A

C_2F_4O (liq) 71HOD
Trifluoroacetyl fluoride
Heat Capacity
Temperature range 14 to 214 K.
Phase Changes
c/liq 113.69 K, ΔH = 4869 J·mol^{-1}
ΔS = 42.83 J·mol^{-1}·K^{-1}
liq/g 214.10 K, ΔH = 19267 J·mol^{-1}
ΔS = 89.99 J·mol^{-1}·K^{-1}
Molecular Weight 116.0150
Wiswesser Line Notation FXFFVF
Evaluation A

$C_2HBrClF_3$ (liq) 84GOL/KOL
2-Bromo-2-chloro-1,1,1-trifluoroethane
Phase Changes
c/liq 157.4 K, ΔH = 4840 J·mol^{-1}
ΔS = 30.7 J·mol^{-1}·K^{-1}
Molecular Weight 197.3821
Wiswesser Line Notation GYEXFFF
Evaluation A

$C_2HBrClF_3$ (liq) 84GOL/KOL
1-Bromo-2-chloro-1,1,2-trifluoroethane
Phase Changes
c/liq 146.2 K, ΔH = 4380 J·mol^{-1}
ΔS = 29.9 J·mol^{-1}·K^{-1}
Molecular Weight 197.3821
Wiswesser Line Notation GYFXFFE
Evaluation A

$C_2HBrClF_3$ (liq) 88VES/ZAB
1-Bromo-2-chloro-1,1,2-trifluoroethane
Heat Capacity 298.15 K, C_p = 160.3 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
C_p(J·mol^{-1}·K^{-1}) = 115.64 + 0.1501(T/K) (298 to 318 K).
Molecular Weight 197.3821
Wiswesser Line Notation GYFXFFE
Evaluation A

$C_2HBrClF_3$ (liq) 88VES/ZAB
2-Bromo-2-chloro-1,1,1-trifluoroethane
Heat Capacity 298.15 K, C_p = 156.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
C_p(J·mol^{-1}·K^{-1}) = 107.69 + 0.1639(T/K) (298 to 318K).
Molecular Weight 197.3821
Wiswesser Line Notation GYEXFFF
Evaluation A

C_2HCl_3 (liq) 84GOL/KOL
Trichloroethene; Trichloroethylene
Phase Changes
c/liq 188.5 K, ΔH = 8450 J·mol^{-1}
ΔS = 44.8 J·mol^{-1}·K^{-1}
Molecular Weight 131.3889
Wiswesser Line Notation GYGU1G
Evaluation A

$C_2HCl_3O_2$ (c) 1895PIC
Trichloroacetic acid
Heat Capacity 289–320 K, C_p = 314 J·mol^{-1}·K^{-1}
Temperature range 289 to 356 K.
Phase Changes
c/liq 332.25 K, ΔH = 5898 J·mol^{-1}
ΔS = 17.75 J·mol^{-1}·K^{-1}
Molecular Weight 163.3877
Wiswesser Line Notation QVXGGG
Evaluation D

$(C_2H_2Cl_2)_n$ (gls) 67LEB/RAB
Polyvinylidene chloride
Heat Capacity 298.15 K, C_p = 83.05 J·mol^{-1}·K^{-1}
Temperature range 58 to 300 K.
Entropy 298.15 K, S = 86.69 J·mol^{-1}·K^{-1}
Molecular Weight 96.9432
Wiswesser Line Notation /*XGG1*/
Evaluation B

$C_2H_2Cl_2O_2$ (liq) 1895PIC
Dichloroacetic acid; Dichloroethanoic acid
Heat Capacity 291–323 K, C_p = 207 J·mol^{-1}·K^{-1}
Temperature range 253 to 323 K.
Phase Changes
c/liq 283.95 K, ΔH = 7644 J·mol^{-1}
ΔS = 26.9 J·mol^{-1}·K^{-1}
Molecular Weight 128.9426
Wiswesser Line Notation QVYGG
Evaluation D

$C_2H_2Cl_4$ (liq) 82KOS/KOL
1,1,2,2-Tetrachloroethane
Heat Capacity 298.15 K, C_p = 165.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S = 244.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 207.3 K, ΔH = 544 J·mol^{-1}
ΔS = 2.62 J·mol^{-1}·K^{-1}
c,I/liq 230.8 K, ΔH = 9172 J·mol^{-1}
ΔS = 39.79 J·mol^{-1}·K^{-1}
Molecular Weight 167.8498
Wiswesser Line Notation GYGYGG
Evaluation A
Data for (c,I).

$C_2H_2Cl_4$ (liq) 82KOS/KOL
1,1,2,2-Tetrachloroethane
Heat Capacity 298.15 K, C_p = 165.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S = 247.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 204.8 K, ΔH = 356 J·mol^{-1}
ΔS = 1.74 J·mol^{-1}·K^{-1}
c,II/liq 230.3 K, ΔH = 9521 J·mol^{-1}
ΔS = 41.51 J·mol^{-1}·K^{-1}
Molecular Weight 167.8498
Wiswesser Line Notation GYGYGG
Evaluation A
Data for (c,II).

$C_2H_2CuO_4{\cdot}4D_2O$ (c) 76MAT/KUM
Copper (II) formate tetradeuterate
Heat Capacity 300.16 K, C_p = 329.69 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 245.64 K, ΔH = 936.9 J·mol^{-1}
ΔS = 3.814 J·mol^{-1}·K^{-1}
Molecular Weight 233.7054
Wiswesser Line Notation OVH 2 .CU &QH4 &14/H-2 8
Evaluation B

$C_2H_2CuO_4{\cdot}4H_2O$ (c) 76MAT/KUM
Copper (II) formate tetrahydrate
Heat Capacity 295.47 K, C_p = 290.20 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 235.78 K, ΔH = 836.0 J·mol^{-1}
ΔS = 3.546 J·mol^{-1}·K^{-1}
Molecular Weight 225.6422
Wiswesser Line Notation OVH 2 .CU &QH4
Evaluation B

C_2H_3Cl (liq) 67LEB/RAB
Vinyl chloride
Heat Capacity 298.15 K, C_p = 89.45 J·mol^{-1}·K^{-1}
Temperature range 58 to 300 K.
Entropy 298.15 K, S = 118.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 119.31 K, ΔH = 4916 J·mol^{-1}
ΔS = 41.2 J·mol^{-1}·K^{-1}
Molecular Weight 62.4987
Wiswesser Line Notation G1U1
Evaluation B

$(C_2H_3Cl)_n$ (c) 55ALF/DOL
Polyvinyl chloride
Heat Capacity 298 K, C_p = 59.47 J·mol^{-1}·K^{-1}
Temperature range 253 to 393 K.
C_p calculated from equation. C_p(cal·g^{-1}·K^{-1}) = 0.2092 + $7.29\times10^{-4}T$, where $T<60$ °C for L-38 PVC.
C_p(cal·g^{-1}·K^{-1}) = 0.2048 + $8.46\times10^{-4}T$, where $T<60$ °C for annealed PVC.
Molecular Weight 62.4984
Wiswesser Line Notation /*YG1*/
Evaluation A
T(glass) = 78.5 °C.

$(C_2H_3Cl)_n$ (gls) 67LEB/RAB
Polyvinyl chloride
Heat Capacity 298.15 K, C_p = 59.96 J·mol^{-1}·K^{-1}
Temperature range 58 to 300 K.
Value per monomer unit.
Entropy 298.15 K, S = 65.10 J·mol^{-1}·K^{-1}
Molecular Weight 62.4984
Wiswesser Line Notation /*YG1*/
Evaluation B

$C_2H_3ClO_2$ (c) 1895PIC
Monochloroacetic acid; Chloroacetic acid
Heat Capacity 288–318 K, C_p = 144 J·mol^{-1}·K^{-1}
Temperature range 288 to 349 K.
Phase Changes
c/liq 334.33 K, ΔH = 16296 J·mol^{-1}
ΔS = 48.74 J·mol^{-1}·K^{-1}
α-Isomer.
c/liq 329.16 K, ΔH = 13933 J·mol^{-1}
ΔS = 42.33 J·mol^{-1}·K^{-1}
β-Isomer.
Molecular Weight 94.4975
Wiswesser Line Notation QV1G
Evaluation D

$C_2H_3Cl_3$ (liq) 82MAR
1,1,1-Trichloroethane; Methylchloroform
Phase Changes
c,II/c,I 224.5 K, ΔH = 7470 J·mol^{-1}
ΔS = 33.3 J·mol^{-1}·K^{-1}
c,I/liq 240.9 K, ΔH = 1550 J·mol^{-1}
ΔS = 6.43 J·mol^{-1}·K^{-1}
Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation C

$C_2H_3Cl_3$ (c) 88MAR/MON
1,1,1-Trichloroethane; Methylchoroform
Heat Capacity 225 K, C_p = 123 J·mol^{-1}·K^{-1}
Temperature range 10 to 225 K. Data given graphically and estimated from graph.
Molecular Weight 133.4047
Wiswesser Line Notation GXGG1
Evaluation A

$C_2H_3LiO_2{\cdot}2H_2O$ (c) 84MEI/GRO
Lithium acetate dihydrate
Heat Capacity 298.15 K, C_p = 169.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 400 K.
Phase Changes
c/aq 324.71 K, ΔH = 24250 J·mol^{-1}
ΔS = 74.7 J·mol^{-1}·K^{-1}
Transition of dihydrate to anhydrous salt and aqueous solution.
Molecular Weight 102.0159
Wiswesser Line Notation OV1 .LI &QH 2
Evaluation B

C_2H_3N (liq) 82MAR
Acetonitrile; Methyl cyanide
Phase Changes
c,II/c,I 218.0 K, ΔH = 800 J·mol^{-1}
ΔS = 3.67 J·mol^{-1}·K^{-1}
c,I/liq 228.7 K, ΔH = 6670 J·mol^{-1}
ΔS = 29.2 J·mol^{-1}·K^{-1}
Molecular Weight 41.0524
Wiswesser Line Notation NC1
Evaluation C

$(C_2H_3NO)_n$ (c) 80FIN/KUM
Polyglycine I
Heat Capacity 298.15 K, C_p = 102.5 J·mol^{-1}·K^{-1}
Temperature range 150 to 375 K.
$C_p = 37.744 + 0.218T - 2.333\times10^{-6}T^2$.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B
Same data as in 81FIN/KUM. β-sheet structure.

$(C_2H_3NO)_n$ (c) 80FIN/KUM
Polyglycine II
Heat Capacity 298.15 K, C_p = 93.46 J·mol^{-1}·K^{-1}
Temperature range 150 to 375 K.
$C_p = 57.598 + 0.05T + 2.357\times10^{-4}T^2$.
Molecular Weight 57.0518
Wiswesser Line Notation /*MV1*/
Evaluation B
Same data as in 81FIN/KUM. 3_1 helical structure.

$C_2H_3N_3$ (c) 89JIM/ROU
1,2,4-Triazole
Heat Capacity 298.15 K, C_p = 78.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 69.0658
Wiswesser Line Notation T5MN DNJ
Evaluation A

$C_2H_3NaO_2$ (c) 83FRA/PLA
Sodium ethanoate; Sodium acetate
Heat Capacity 298.15 K, C_p = 100.83 J·mol^{-1}·K^{-1}
Temperature range 7 to 350 K.
Entropy 298.15 K, S = 138.10 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 21 K, ΔS = 12.5 J·mol^{-1}·K^{-1}
Questionable second-order transition.
Molecular Weight 82.0343
Wiswesser Line Notation OV1 .NA
Evaluation A

$C_2H_3NaO_2{\cdot}3H_2O$ (c) 84MEI/GRO
Sodium acetate trihydrate
Heat Capacity 298.15 K, C_p = 229.0 J·mol^{-1}·K^{-1}
Temperature range 270 to 400 K.
Phase Changes
c/aq 331.52 K, ΔH = 37860 J·mol^{-1}
ΔS = 114.2 J·mol^{-1}·K^{-1}
Transition of trihydrate to anhydrous salt and aqueous solution.
Molecular Weight 136.0799
Wiswesser Line Notation OV1 .N*A* &QH 3
Evaluation B

$C_2H_3O_2Tl$ (c) 76MEI/SEY
Thallium acetate
Phase Changes
c,I/liq 404 K, ΔH = 17573 J·mol^{-1}
ΔS = 43.5 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 263.4145
Wiswesser Line Notation OV1 .TL
Evaluation B

C_2H_4 (liq) 37EGA/KEM
Ethylene
Heat Capacity 170 K, C_p = 67.24 J·mol^{-1}·K^{-1}
Temperature range 15 to 170 K.
Phase Changes
c/liq 103.95 K, ΔH = 3351 J·mol^{-1}
ΔS = 32.23 J·mol^{-1}·K^{-1}
liq/g 169.40 K, ΔH = 13544 J·mol^{-1}
ΔS = 79.95 J·mol^{-1}·K^{-1}
Molecular Weight 28.0536
Wiswesser Line Notation 1U1
Evaluation B

C_2H_4 (liq) 83CHA/HAL
Ethylene
Heat Capacity 170 K, C_p = 67.4 J·mol^{-1}·K^{-1}
Temperature range 16 to 169 K.
Entropy 170 K, S = 117.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 103.97 K, ΔH = 3351 J·mol^{-1}
ΔS = 32.23 J·mol^{-1}·K^{-1}
Molecular Weight 28.0536
Wiswesser Line Notation 1U1
Evaluation A
A reevaluation of the original measured data from: 37EGA/KEM.

$C_2H_4Br_2$ (liq) 65FIN/GRU
1,2-Dibromoethane; Ethylene dibromide
Heat Capacity 300 K, C_p = 136.4 J·mol^{-1}·K^{-1}
Molecular Weight 187.8616
Wiswesser Line Notation E2E
Evaluation B

$C_2H_4Cl_2$ (liq) 85LAI/ROU
1,2-Dichloroethane; Ethylene dichloride
Heat Capacity 298.15 K, C_p = 128.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.9596
Wiswesser Line Notation G2G
Evaluation B

$C_2H_4F_2$ (liq) 82POR/PON
Freon 152A; 1,1-Difluoroethane; Ethylidene difluoride
Heat Capacity 298.17 K, C_p = 118.4 J·mol^{-1}·K^{-1}
Temperature range 220 to 425 K.
Unsmoothed experimental datum.
C_p data given as 1.793 J·g^{-1}·K^{-1}.
Molecular Weight 66.0504
Wiswesser Line Notation FYF1
Evaluation C

$C_2H_4N_2O_2$ (c) 83LEB/KAT
Diformylhydrazine
Heat Capacity 298.15 K, C_p = 99.12 J·mol^{-1}·K^{-1}
Temperature range 298 to 350 K.
C_p = 0.908 x 10^{-4} T^3 − 0.0923 T^2 + 31.3779 T − 3457.8187 J·mol^{-1}·K^{-1} (298 to 350 K).
Molecular Weight 88.0658
Wiswesser Line Notation VHMMVH
Evaluation B

C_2H_4O (liq) 88LEB/VAS
Ethanal
Heat Capacity 298.15 K, C_p = 89.05 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S = 117.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 149.78 K, ΔH = 2310 J·mol^{-1}
ΔS = 15.43 J·mol^{-1}·K^{-1}
liq/liq 242.9 K, ΔH = 1716 J·mol^{-1}
ΔS = 7.35 J·mol^{-1}·K^{-1}
Lambda type transition.
Molecular Weight 44.0530
Wiswesser Line Notation VH1
Evaluation A

$(C_2H_4O)_n$ (c) 57SOC/TRA
Polyvinyl alcohol
Heat Capacity 245 K, C_p = 45.9 J·mol^{-1}·K^{-1}
Temperature range 58 to 245 K;
C_p value is unsmoothed experimental datum.
Molecular Weight 44.0530
Wiswesser Line Notation /*QY1*/
Evaluation B
See also 62WAR/BRO

$(C_2H_4O)_n$ (liq) 82ZAR
Polyethylene glycol
Heat Capacity 298 K, C_p = 1314 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K
Molecular Weight 600
Wiswesser Line Notation /*O2*/
Evaluation B

$(C_2H_4O)_n$ (liq) 82ZAR
Polyethylene glycol
Heat Capacity 323 K, C_p = 3346 J·mol^{-1}·K^{-1}
Temperature range 323, 363 K.
Molecular Weight 1500
Wiswesser Line Notation /*O2*/
Evaluation B

$C_2H_4O{\cdot}7H_2O$ (c) 82LEA/MUR
Ethylene oxide hydrate
Heat Capacity
Temperature range 120 to 260 K. Data given graphically.
Phase Changes
c/liq 283.2 K, ΔH = 48000 J·mol^{-1}
ΔS = 169.5 J·mol^{-1}·K^{-1}
Molecular Weight 170.1594
Wiswesser Line Notation T3OTJ &QH 7
Evaluation A
Actual formula: $C_2H_4O{\cdot}6.89H_2O$

$C_2H_4O_2$ (liq) 1895PIC
Acetic acid; Ethanoic acid
Heat Capacity 287–335 K, C_p = 137 J·mol^{-1}·K^{-1}
Temperature range 260 to 335 K.
Phase Changes
c/liq 290.06 K, ΔH = 11126 J·mol^{-1}
ΔS = 38.36 J·mol^{-1}·K^{-1}
Molecular Weight 60.0524
Wiswesser Line Notation QV1
Evaluation D

$C_2H_4O_2$ (liq) 1881BER/OGI
Methyl formate; Methyl methanoate
Heat Capacity 298 K, C_p = 130 J·mol^{-1}·K^{-1}
Temperature range 286 to 302 K.
C_p given as 0.516 cal·g^{-1}·K^{-1}.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation D

$C_2H_4O_2$ (liq) 87ZAB/HYN
Methyl formate; Methyl methanoate
Heat Capacity 298.75 K, C_p = 120.57 J·mol^{-1}·K^{-1}
Temperature range 293 to 299 K.
Unsmoothed experimental datum.
Molecular Weight 60.0524
Wiswesser Line Notation VHO1
Evaluation B

C_2H_5NO (liq) 76SKO/SUU
N-Methylformamide; N-Methylmethanamide
Heat Capacity 298.15 K, C_p = 123.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation VHM1
Evaluation A

C_2H_5NO (c) 76SKO/SUU
Acetamide; Ethanamide
Heat Capacity 298.15 K, C_p = 90.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A

C_2H_5NO (c) 83DEW/DEK
Acetamide; Ethanamide
Heat Capacity 300 K, C_p = 90.00 J·mol^{-1}·K^{-1}
Temperature range 90 to 360 K.
Phase Changes
c/liq 353.33 K, ΔH = 15590 J·mol^{-1}
ΔS = 44.1 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation B(C_p), A(Phase changes).

C_2H_5NO (c) 84NUR/BER
Acetamide; Ethanamide
Heat Capacity 298.15 K, C_p = 91.27 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 115.0 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A

C_2H_5NO (c) 86EMO/NAU
Acetamide; Ethanamide
Heat Capacity 298 K, C_p = 86.65 J·mol^{-1}·K^{-1}
Temperature range 298 to 400 K.
C_p data given at 298 K as 1.467 kJ·kg^{-1}·K^{-1} (extrapolated).
C_p = 1.481 + 0.0069(T−300) kJ·kg^{-1}·K^{-1} (300 to 330).
Phase Changes
c/liq 353.5 K, ΔH = 15606 J·mol^{-1}
ΔS = 44.15 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation B(C_p), A(Phase changes)
Stable form.

C_2H_5NO (c) 86EMO/NAU
Acetamide; Ethanamide
Phase Changes
c/liq 342.15 K, ΔH = 12522 to 12877 J·mol^{-1}
ΔS = 36.6 to 37.6 J·mol^{-1}·K^{-1}
Molecular Weight 59.0676
Wiswesser Line Notation ZV1
Evaluation A
Unstable form.

$C_2H_5NO_2$ (c) 76BER/BOU
Methyl carbamate
Phase Changes
c/liq 328.6 K, ΔH = 16700 J·mol^{-1}
ΔS = 51.0 J·mol^{-1}·K^{-1}
Molecular Weight 75.0672
Wiswesser Line Notation ZVO1
Evaluation A

$C_2H_5NO_4$·0.5H_2O (c) 89FUK/MAT
Ammonium hydrogen oxalate hemihydrate
Heat Capacity 298.15 K C_p = 166.91 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K
Entropy 298.15 K S = 189.24 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 145.4 K ΔH = 0.37 J mol^{-1}
ΔS = 3.01 J·mol^{-1}·K^{-1}
Order − disorder transition
Molecular Weight 116.0734
Wiswesser Line Notation ZH QVVQ &QH 0.5
Evalation A

$C_2D_5NO_4$·0.5D_2O (c) 89FUK/MAT
Ammonium hydrogen oxalate hemihydrate-*d*6
Heat Capacity 298.15 K C_p =179.97 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K
Entropy 298.15 K S = 204.45 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 160.1 K ΔH =0.56 J mol^{-1}
ΔS =4.12 J·mol^{-1}·K^{-1}
Order-disorder transition
Molecular Weight 122.1208
Wiswesser Line Notation
ZH QVVQ &QH 0.5 &1/H-2 2 &2/4/7/10/11/H-2
Evaluation A

C_2H_5NS (c) 82SAB/TOR
Thioacetamide
Heat Capacity 298 K, C_p = 100.3 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.335 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, ΔH = 82800 J·mol^{-1}
ΔS = 277.7 J·mol^{-1}·K^{-1}
Molecular Weight 75.1282
Wiswesser Line Notation ZY1&US
Evaluation B

C_2H_6 (liq) 76ATA/CHI
Ethane
Heat Capacity 100 K, C_p = 68.66 J·mol^{-1}·K^{-1}
Temperature range 50 to 100 K.
Data given graphically.
C_p = 0.69933 (T/K)− 2.385 J·mol^{-1}·K^{-1} (50 to 70 K, for solid).
Phase Changes
c,II/c,I 89.813 K, ΔH = 2282 J·mol^{-1}
ΔS = 25.48 J·mol^{-1}·K^{-1}
c/liq 90.341 K, ΔH = 583 J·mol^{-1}
ΔS = 6.46 J·mol^{-1}·K^{-1}
Triple point.
Molecular Weight 30.0694
Wiswesser Line Notation 2H
Evaluation A

$C_2H_6Cl_2Si$ (liq) 71SAM/KOS2
Dichlorodimethylsilane
Heat Capacity 298.15 K, C_p = 171.5 J·mol^{-1}·K^{-1}
Temperature range 21 to 299 K.
Data deposited VINITI, No 2423-71, 17 December, 1970.
C_p(liq) = 18.5676 + 0.06453T + 283310T^{-2}
(198.99 to 300 K) cal·mol^{-1}·K^{-1}.
Entropy 298.15 K, S = 270.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 198.99 K, ΔH = 8828 J·mol^{-1}
ΔS = 44.39 J·mol^{-1}·K^{-1}
Molecular Weight 129.0609
Wiswesser Line Notation G-SI-G1&1
Evaluation A
T_{Debye} = 100.37 K.

$C_2H_6Cl_4D_6MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(deuteromethylammonium)
manganese II
Phase Changes
c,II/c,I 258 K, ΔH = 2.6 J·mol^{-1}
ΔS = 0.007 J·mol^{-1}·K^{-1}
c,I/liq 389 K, ΔH = 14.6 J·mol^{-1}
ΔS = 0.036 J·mol^{-1}·K^{-1}
Molecular Weight 266.9278
Wiswesser Line Notation ZH&1 2 .MN G4 &1/H-2 3
Evaluation A

$C_2H_6N_2O$ (c) 87DEL/FER
Methylurea; Monomethylurea
Phase Changes
c/liq 373.8 K, ΔH = 15750 J·mol^{-1}
ΔS = 42.1 J·mol^{-1}·K^{-1}
Molecular Weight 74.0822
Wiswesser Line Notation ZVM1
Evaluation A

$C_2H_6N_2O_4$ (c) 86MAT/SUG
Hydrazinium hydrogen oxalate
Heat Capacity 299.47 K, C_p = 157.6 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Value is unsmoothed experimental datum.
Phase Changes
c,II/c,I 217.6 K, ΔH = 1090 J·mol^{-1}
ΔS = 4.18 J·mol^{-1}·K^{-1}
Molecular Weight 122.0804
Wiswesser Line Notation QVVQ &ZZ
Evaluation A

C_2H_6O (liq) 40MAZ
Ethanol; Ethyl alcohol
Heat Capacity 297.8 K, C_p = 114.7 J·mol^{-1}·K^{-1}
Temperature range 174 to 298 K.
Unsmoothed experimental datum.
C_p(liq) = 0.5437 + 0.001858t + 0.0000098t^2 cal·g^{-1}·°C^{-1}.
C_p(298.15 K) = 114.9 J·mol^{-1}·K^{-1}, calculated from equation.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 44YOS
Ethanol; Ethyl alcohol
Phase Changes
c/liq 159 K, ΔH = 4973 J·mol^{-1}
ΔS = 31.3 J·mol^{-1}·K^{-1}
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 76FOR/BEN2
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p = 112.094 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A
Data from 76FOR/BEN.

C_2H_6O (liq) 77VES/SVO
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p = 112.30 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 82VIL/CAS
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p = 113.75 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 84STE/OLS
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p = 115.9 J·mol^{-1}·K^{-1}
Temperature range 266 to 318 K. C_p given as 0.6011 cal·g^{-1}·C^{-1}.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation B

C_2H_6O (liq) 84ZEG/SOM
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p = 112.67 J·mol^{-1}·K^{-1}
One temperature
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

C_2H_6O (liq) 86TAN/TOY
Ethanol; Ethyl alcohol
Heat Capacity 298.15 K, C_p = 112.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 46.0688
Wiswesser Line Notation Q2
Evaluation A

$(C_2H_6OSi)_n$ (liq) 78LEB/MUK
Poly(dimethylsiloxane)
Heat Capacity 298.15 K, C_p = 117.8 J·mol^{-1}·K^{-1}
Temperature range 8 to 332 K.
Entropy 298.15 K, S = 154.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 246 K, ΔH = 4540 J·mol^{-1}
ΔS = 18.6 J·mol^{-1}·K^{-1}
Degree of crystallinity is 67%.
Molecular Weight 74.1543
Wiswesser Line Notation /*-SI-O*1&1/
Evaluation A

$C_2H_6O_2$ (liq) 01FOR
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity C_p = 152 J·mol^{-1}·K^{-1}
Temperature range 286 to 332.7 K.
Value given over temperature range.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation D

$C_2H_6O_2$ (liq) 82ZAR
Ethylene glycol; 1,2-Dihydroxyethane; 1,2-Ethanediol
Heat Capacity 298 K, C_p = 149.8 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 62.0682
Wiswesser Line Notation Q2Q
Evaluation B

C_2H_6Zn (liq) 84SHE/NIS
Dimethyl zinc
Heat Capacity 298.15 K, C_p = 129.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 201.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 210.26 K, ΔH = 1061 J·mol^{-1}
ΔS = 5.05 J·mol^{-1}·K^{-1}
c,I/liq 230.13 K, ΔH = 6830 J·mol^{-1}
ΔS = 29.67 J·mol^{-1}·K^{-1}
Molecular Weight 95.4494
Wiswesser Line Notation 1-ZN-1
Evaluation A

$C_2H_8N_2$ (liq) 51AST/JAN
N,N'-Dimethylhydrazine
Heat Capacity 298.15 K, C_p = 171.04 J·mol^{-1}·K^{-1}
Temperature range 15 to 298 K.
Entropy 298.15 K, S = 199.15 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 264.28 K, ΔH = 13638 J·mol^{-1}
ΔS = 51.60 J·mol^{-1}·K^{-1}
Molecular Weight 60.0986
Wiswesser Line Notation 1MM1
Evaluation A

$C_2H_8N_2$ (liq) 88BOB/KAM
1,2-Diaminoethane; Ethylenediamine
Heat Capacity 313 K, C_p = 170 J·mol^{-1}·K^{-1}
Temperature range 313 to 413 K
Molecular Weight 60.0986
Wiswesser Line Notation Z2Z
Evaluation D

$C_2H_{12}B_{10}$ (liq) 81GOR/ZAL

m-Carborane; 1,7-Carborane-12

Heat Capacity 298.15 K, C_p = 229.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.

Entropy 298.15 K, S = 211.8 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II	58.0 K,	ΔH = 41 J·mol^{-1}
		ΔS = 0.73 J·mol^{-1}·K^{-1}
c,II/c,I	165 K,	ΔH = 1903 J·mol^{-1}
		ΔS = 9.50 J·mol^{-1}·K^{-1}
c,I/liq	280.1 K,	ΔH = 4326 J·mol^{-1}
		ΔS = 14.8 J·mol^{-1}·K^{-1}

Molecular Weight 144.2168
Wiswesser Line Notation
Evaluation A

$C_2H_{12}Br_6N_2Te$ (c) 86ONO/MAT

Bis(methylammonium) hexabromotellurate (IV)

Heat Capacity 298.15 K, C_p = 314.70 J·mol^{-1}·K^{-1}
Temperature range 13 to 320 K.

Entropy 298.15 K, S = 592.98 J·mol^{-1}·K^{-1}

Phase Changes

c,IV/c,III	129.0 K,	ΔH = 1677 J mol^{-1}
		ΔS = 13.0 J·mol^{-1}·K^{-1}
c,III/c,II	163.9 K,	ΔH = 885 J·mol^{-1}·K−1
		ΔS = 5.4 J·mol^{-1}·K^{-1}
c,II/c,I	288.9 K,	ΔH = 4594 J·mol^{-1}
		ΔS = 15.9 J·mol^{-1}·K^{-1}

Molecular Weight 671.1542
Wiswesser Line Notation ZH&1 2 -TE- E6
Evaluation A

$C_2H_{12}Cl_4MnN_2$ (c) 75BOC/ARR

Tetrachlorobis-(methylammonium) manganese II

Phase Changes

c,III/c,II	257 K,	ΔH = 4.8 J·mol^{-1}
		ΔS = 0.017 J·mol^{-1}·K^{-1}
c,II/c,I	393 K,	ΔH = 3.6 J·mol^{-1}
		ΔS = 0.007 J·mol^{-1}·K^{-1}

Molecular Weight 260.8802
Wiswesser Line Notation ZH&1 2 -MN- G4
Evaluation A

$C_2H_{12}Cl_6Te$ (c) 88ONO/MAT

Methylammonium hexachlorotellurate

Heat Capacity 298.21 K, C_p = 314.9 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Unsmoothed experimental datum.

Phase Changes

c,VI/c,V	73.0 K,	ΔH = 470 J·mol^{-1}
		ΔS = 6.4 J·mol^{-1}·K^{-1}
c,V/c,IV	136.8 K,	ΔH = 1810 J·mol^{-1}
		ΔS = 14.9 J·mol^{-1}·K^{-1}
	Lambda type transition.	
c,IV/c,III	155 K,	ΔH = 390 J·mol^{-1}
		ΔS = 2.5 J·mol^{-1}·K^{-1}
c,III/c,II	226.0 K,	ΔH = 330 J·mol^{-1}
		ΔS = 1.7 J·mol^{-1}·K^{-1}
c,II/c,I	439 K,	ΔH = 4400 J·mol^{-1}
		ΔS = 9.8 J·mol^{-1}·K^{-1}

Molecular Weight 376.4348
Wiswesser Line Notation ZH&1 2 -TE- G4
Evaluation B(C_p), A(Phase changes)

$C_2H_{12}I_6N_2Te$ (c) 86ONO/MAT

Bis(methylammonium) hexaiodotellurate

Heat Capacity 298.15 K, C_p = 307.05 J·mol^{-1}·K^{-1}
Temperature Range 12 to 300 K

Entropy 298.15 K, S = 639.71 mol^{-1}K^{-1}

Phase Changes

c,III/c,II	66.1 K,	ΔH = 403 J·mol^{-1}·K^{-1}
		ΔS = 6.1 *J* mol-1K^{-1}
c,II/c,I	115.6 K,	ΔH = 2555 J·mol^{-1}
		ΔS = 22.1 J·mol^{-1}·K^{-1}

Molecular Weight 718.1547
Wiswesser Line Notation ZH&1 2 -TE- I6
Evaluation A

$C_3H_2N_2$ (c) 87WAS/OLE

Malononitrile

Heat Capacity
Temperature range 150 to 320 K.
Data given graphically.

Phase Changes

c,IV/c,II	140 K	
	Re-entrant phase transition; second order.	
c,III/c,II		
	First order transition; slow.	
c,I/c,I′	303 K	
	First order transition.	
c,III/c,II	260 K	
	Phase III is stable below 260 K.	
c,II/c,I	295 K	
	Second order transition.	

Molecular Weight 66.0622
Wiswesser Line Notation NC1CN
Evaluation A

$C_3H_3Cl_3$ (liq) 84GOL/KOL

1,1,2-Trichloroethane

Phase Changes

c/liq	237.9 K,	ΔH = 10880 J·mol^{-1}
		ΔS = 45.7 J·mol^{-1}·K^{-1}

Molecular Weight 145.4157
Wiswesser Line Notation GYG1G
Evaluation A

$C_3H_3N_3O_3$ (c) 83DEW/DEK

Cyanuric acid; Triazine triol

Heat Capacity 300 K, C_p = 133.63 J·mol^{-1}·K^{-1}
Temperature range 90 to 340 K.
C_p = 20.63 + 0.3758 (T/K) J·mol^{-1}·K^{-1} (90 to 340 K).

Molecular Weight 129.0750
Wiswesser Line Notation T6N CN ENJ BQ DQ FQ
Evaluation B(C_p), A(Phase changes).

$C_3H_4Cl_3Si$ (c) 75KOS/SAM

β-Trichlorosilylpropionitrile

Heat Capacity 298.15 K, C_p = 186.1 J·mol^{-1}·K^{-1}
Temperature range 13.4 to 322.5 K.
Deposited in VINITI, No 586–75, 10 March 1975.

Entropy 298.15 K, S = 246.0 J·mol^{-1}·K^{-1}

Phase Changes

c/liq	307.90 K,	ΔH = 21242 J·mol^{-1}
		ΔS = 69.0 J·mol^{-1}·K^{-1}

Molecular Weight 174.5091
Wiswesser Line Notation NC2-SI-GGG
Evaluation A

$C_3H_4N_2$ (c) 83DEW/DEK
Imidazole
Heat Capacity 300 K, C_p = 89.78 J·mol^{-1}·K^{-1}
Temperature range 90 to 370 K.
Phase Changes
c/liq 362.69 K, ΔH = 12821 J·mol^{-1}
ΔS = 35.35 J·mol^{-1}·K^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation B(C_p), A(Phase changes).

$C_3H_4N_2$ (c) 83DEW/OFF
Imidazole
Heat Capacity 310 K, C_p = 94.4 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 361.9 K, ΔH = 12800 J·mol^{-1}
ΔS = 35.37 J·mol^{-1}·K^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation B

$C_3H_4N_2$ (c) 87JIM/ROU
Imidazole
Heat Capacity 298.15 K, C_p = 82.4 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.21 J·K^{-1}·g^{-1}.
Molecular Weight 68.0780
Wiswesser Line Notation T5M CNJ
Evaluation B

$C_3H_4N_2$ (c) 83DEW/OFF
Pyrazole
Heat Capacity 300 K, C_p = 87.9 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 333.1 K, ΔH = 13800 J·mol^{-1}
ΔS = 41.43 J·mol^{-1}·K^{-1}
Molecular Weight 68.0780
Wiswesser Line Notation T5MNJ
Evaluation B

$C_3H_4N_2$ (c) 87JIM/ROU
Pyrazole
Heat Capacity 298.15 K, C_p = 81.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.19 J·K^{-1}·g^{-1}.
Molecular Weight 68.0780
Wiswesser Line Notation T5MNJ
Evaluation B

$C_3H_4N_2O$ (c) 83DEW/OFF
Cyanoacetamide
Heat Capacity 300 K, C_p = 111.1 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c,II/c,I 346.5 K, ΔH = 1200 J·mol^{-1}
ΔS = 3.46 J·mol^{-1}·K^{-1}
c,I/liq 387.3 K, ΔH = 21700 J·mol^{-1}
ΔS = 56.0 J·mol^{-1}·K^{-1}
Molecular Weight 84.0774
Wiswesser Line Notation ZV1CN
Evaluation B

$C_3H_4O_2$ (liq) 83KAR/ABD2
Acrylic acid
Heat Capacity 300 K, C_p = 145.70 J·mol^{-1}·K^{-1}
Temperature range 290 to 344 K.
C_p given as 2021.8 J·kg^{-1}·K^{-1}.
Molecular Weight 72.0634
Wiswesser Line Notation QV1U1
Evaluation B

$C_3H_4O_2$ (liq) 85KAR/ABD2
Acrylic acid
Phase Changes
c/liq 285.7 K, ΔH = 9509.7 J·mol^{-1}
ΔS = 33.3 J·mol^{-1}·K^{-1}
Molecular Weight 72.0634
Wiswesser Line Notation QV1U1
Evaluation A

$C_3H_4O_2$ (liq) 83LEB/YEV
β-Propiolactone
Heat Capacity 298.15 K, C_p = 122.1 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S = 175.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.86 K, ΔH = 9410 J·mol^{-1}
ΔS = 39.23 J·mol^{-1}·K^{-1}
Molecular Weight 72.0634
Wiswesser Line Notation T4OVTJ
Evaluation A

$C_3H_5KO_2$ (c) 84FRA/WES
Potassium propionate
Heat Capacity 298.15 K, C_p = 129.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S = 142.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 255 K, ΔH = 515 J·mol^{-1}
ΔS = 2.02 J·mol^{-1}·K^{-1}
c,II/c,I 352.5 K
c,I/liq 638.3 K
Molecular Weight 112.1696
Wiswesser Line Notation OV2 .KA
Evaluation A

$C_3H_5LiO_2$ (c) 84FRA/WES
Lithium propionate
Heat Capacity 298.15 K, C_p = 143.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 600 K.
Entropy 298.15 K, S = 175.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 514 K
c,I/liq 606.8 K
Molecular Weight 80.0123
Wiswesser Line Notation OV2 .LI
Evaluation A

$C_3H_5NO_4$ (liq) 81LEB/RYA
Methyl ester of nitroacetic acid;
Methyl nitroacetate
Heat Capacity C_p = 205.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 343 K. Data given over temperature range.
Molecular Weight 119.0768
Wiswesser Line Notation WN1VO1
Evaluation B

$C_3H_5NaO_2$ (c) 83FRA/WES
Sodium propanoate
Heat Capacity 298.15 K, C_p = 134.4 J·mol^{-1}·K^{-1}
Temperature range 9 to 580 K.
Entropy 298.15 K, S = 152.1 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 467.00 K, ΔH = 3209 J·mol^{-1}
ΔS = 6.87 J·mol^{-1}·K^{-1}
c,II/c,I 491.00 K, ΔH = 4357 J·mol^{-1}
ΔS = 8.87 J·mol^{-1}·K^{-1}
c,I/liq 561.91 K, ΔH = 13280.0 J·mol^{-1}
ΔS = 23.63 J·mol^{-1}·K^{-1}
Molecular Weight 96.0611
Wiswesser Line Notation OV2 .NA
Evaluation A

$C_3H_5O_2Tl$ (c) 76MEI/SEY
Thallium propionate
Phase Changes
c,II/c,I 365 K, ΔH = 377 J·mol^{-1}
ΔS = 1.05 J·mol^{-1}·K^{-1}
c,I/liq 468 K, ΔH = 9205 J·mol^{-1}
ΔS = 20.1 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 277.4413
Wiswesser Line Notation OV2 .TL
Evaluation B

$C_3H_5O_2Tl$ (c) 84FER/LOP
Thallium propionate
Heat Capacity 320 K, C_p = 158 J·mol^{-1}·K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,II/c,I 364.8 K, ΔH = 316 J·mol^{-1}
ΔS = 0.83 J·mol^{-1}·K^{-1}
c,I/liq 468.0 K, ΔH = 10476 J·mol^{-1}
ΔS = 22.5 J·mol^{-1}·K^{-1}
Molecular Weight 277.4413
Wiswesser Line Notation OV2 .TL
Evaluation A

C_3H_6 (liq) 39POW/GIA
Propylene; Propene
Heat Capacity 230 K, C_p = 92.09 J·mol^{-1}·K^{-1}
Temperature range 14 to 225 K.
Phase Changes
c/liq 87.85 K, ΔH = 3002 J·mol^{-1}
ΔS = 34.18 J·mol^{-1}·K^{-1}
liq/g 225.35 K, ΔH = 18418 J·mol^{-1}
ΔS = 81.73 J·mol^{-1}·K^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation 2U1
Evaluation B

C_3H_6 (liq) 50AUE/SAG
Propylene, Propene
Heat Capacity 300 K, C_p = 98.9 J·mol^{-1}·K^{-1}
Temperature range 300 to 344 K.
Datum at 80 °C is C_p at the bubble point, 0.5615 Btu(lb)$^{-1}$(°R)$^{-1}$.
Molecular Weight 42.0804
Wiswesser Line Notation 2U1
Evaluation A

C_3H_6 (liq) 83CHA/HAL
Propylene; Propene
Heat Capacity 298.15 K, C_p = 102 J·mol^{-1}·K^{-1}
Temperature range 14 to 340 K.
Entropy 298.15 K, S = 195.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 87.85 K, ΔH = 3003 J·mol^{-1}
ΔS = 34.18 J·mol^{-1}·K^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation 2U1
Evaluation A
A reevaluation of the original measured data from:
31HUF/PAR, 39POW/GIA, 50AUE/SAG.

$(C_3H_6)_n$ (c) 84GRE/LAU
Polypropylene, isotatic, crystalline
Heat Capacity 298.15 K, C_p = 68.99 J·mol^{-1}·K^{-1}
Temperature range 0 to 500 K.
Entropy 298.15 K, S = 69.92 J·mol^{-1}·K^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation A
Glassy transitions range from 260 to 380 K for 51% crystallinity. T(glass) at 260, 272, and 325 K.

$(C_3H_6)_n$ (gls) 84GRE/LAU
Polypropylene, isotatic, amorphous
Heat Capacity 298.15 K, C_p = 88.07 J·mol^{-1}·K^{-1}
Temperature range 0 to 500 K.
Entropy 298.15 K, S = 80.79 J·mol^{-1}·K^{-1}
Molecular Weight 42.0804
Wiswesser Line Notation /*Y1&1*/
Evaluation A
Conformationally disordered crystal to monoclinic crystal at 380 K, ΔH = 600 J·mol^{-1} (38% crystallinity).

$C_3H_6Cl_2Si$ (liq) 71GEI/DZH
Dichloromethylvinylsilane
Heat Capacity 298.15 K, C_p = 177.9 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Deposited in VINITI, No 2722-71, 25 March 1971.
Entropy 298.15 K, S = 381.3 J·mol^{-1}·K^{-1}
Molecular Weight 141.0719
Wiswesser Line Notation G-SI-G1&1U1
Evaluation A

$C_3H_6N_2O_4$ (c) 78GOD/RAC
2,2-Dinitropropane
Heat Capacity 300 K, C_p = 205 J·mol^{-1}·K^{-1}
Temperature range 100 to 347 K.
C_p estimated from graph.
Phase Changes
c,III/c,II 259.67 K, ΔH = 1870 J·mol^{-1}
ΔS = 7.20 J·mol^{-1}·K^{-1}
c,II/c,I 267.7 K, ΔH = 11276 J·mol^{-1}
ΔS = 42.13 J·mol^{-1}·K^{-1}
c,I/liq 324.5 K, ΔH = 2636 J·mol^{-1}
ΔS = 8.12 J·mol^{-1}·K^{-1}
Molecular Weight 134.0914
Wiswesser Line Notation WNX1&1&NW
Evaluation D(C_p), B(Phase changes)

C_3H_6O (liq) 82TAN/ZHO
Propylene oxide; 2-Methyloxirane
Heat Capacity 300 K, C_p = 122.19 J·mol^{-1}·K^{-1}
Temperature range 170 to 325 K.
Molecular Weight 58.0798
Wiswesser Line Notation T3OTJ B1
Evaluation B

C_3H_6O·17H_2O (c) 85HAN
Propylene oxide clathrate hydrate
Heat Capacity 260 K, C_p = 718 J·mol^{-1}·K^{-1}
Temperature range 95 to 260 K.
Phase Changes
c/liq 268.6 K, ΔH = 92700 J·mol^{-1}
ΔS = 345.1 J·mol^{-1}·K^{-1}
Molecular Weight 364.3382
Wiswesser Line Notation T3OTJ B1 &QH 17
Evaluation A

C_3H_6O (liq) 84VAS/PET
Propanal; Propaldehyde
Heat Capacity 298.15 K, C_p = 159.1 J·mol^{-1}·K^{-1}
Temperature range 15 to 335 K.
Entropy 298.15 K, S = 212.90 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 171.32 K, ΔH = 8590 J·mol^{-1}
Molecular Weight 58.0798
Wiswesser Line Notation VH2
Evaluation A

$C_3H_6O_2$ (liq) 69CLE/MEL
1,3-Dioxolan
Heat Capacity
Temperature range 80 to 390 K.
Entropy 298.15 K, S = 280.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 142.4 K, ΔH = 2677 J·mol^{-1}
ΔS = 18.8 J·mol^{-1}·K^{-1}
c,I/liq 175.93 K, ΔH = 6567 J·mol^{-1}
ΔS = 37.3 J·mol^{-1}·K^{-1}
Molecular Weight 74.0792
Wiswesser Line Notation T5O COTJ
Evaluation B

$C_3H_6O_2$·17H_2O (liq) 85HAN
1,3-Dioxolane clathrate hydrate
Heat Capacity 260 K, C_p = 731 J·mol^{-1}·K^{-1}
Temperature range 95 to 260 K.
Phase Changes
c/liq 270.5 K, ΔH = 99100 J·mol^{-1}
ΔS = 366.4 J·mol^{-1}·K^{-1}
Molecular Weight 380.3376
Wiswesser Line Notation T5O COTJ &QH 17
Evaluation A

$C_3H_6O_2$ (liq) 82BIR/SIK
Propionic acid; Propanoic acid
Heat Capacity 298.15 K, C_p = 158.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K.
Equation only.
$C_p = 129.7 - 0.1263\ T + 0.0007486\ T^2$ J·mol^{-1}·K^{-1}.
Molecular Weight 74.0792
Wiswesser Line Notation QV2
Evaluation C

$(C_3H_6O_2)_n$ (c) 69CLE/MEL
Poly-1,3-dioxolan
Heat Capacity 298.15 K, C_p = 113.1 J·mol^{-1}·K^{-1}
Temperature range 80 to 390 K. Extrapolated data.
Entropy 298.15 K, S = 112.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 209 K
Glass transition.
c,I/liq 325 K, ΔH = 16698 J·mol^{-1}
ΔS = 5.14 J·mol^{-1}·K^{-1}
Molecular Weight 74.0792
Wiswesser Line Notation /*1O1O1*/
Evaluation B

$C_3H_6O_3$ (liq) 44YOS
2-Hydroxypropanoic acid (DL); Lactic acid (DL)
Phase Changes
c/liq 290 K, ΔH = 11344 J·mol^{-1}
ΔS = 39.1 J·mol^{-1}·K^{-1}
Molecular Weight 90.0786
Wiswesser Line Notation QY1&VQ -DL
Evaluation B

$C_3H_6O_3$ (c) 68CLE/MEL
1,3,5-Trioxane
Heat Capacity 298.15 K, C_p = 111.4 J·mol^{-1}·K^{-1}
Temperature range 80 to 310 K.
Entropy 298.15 K, S = 133.0 J·mol^{-1}·K^{-1}
Molecular Weight 90.0786
Wiswesser Line Notation T6O CO EOTJ
Evaluation B

$C_3H_6O_3$ (liq) 83SAN/CIO
Methylene glycol acetate
Heat Capacity 298.15 K C_p = 214 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K.
$C_p°$ (kJ kg−1K−1) = 0.033053T − 7.401
Molecular Weight 87.0549
Wiswesser Line Notation Q1OV1
Evaluation D

C_3H_7NO (liq) 82VOR/YAK
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p = 150.5 J·mol^{-1}·K^{-1}
Temperature range 297.15 to 299.15 K.
C_p given as 2.059 J·K^{-1}·g^{-1}.
Molecular Weight 73.0944
Wiswesser Line Notation VHN1&1
Evaluation B

C_3H_7NO (liq) 84ZEG/SOM
N,N-Dimethylformamide; N,N-Dimethylmethanamide; DMF
Heat Capacity 298.15 K, C_p = 148.36 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 61.0834
Wiswesser Line Notation VHN1&1
Evaluation B

$C_3H_7NO_2$ (c) 83SKO/SAB
3-Aminopropanoic acid
Heat Capacity 298 K, C_p = 116.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 89.0938
Wiswesser Line Notation Z2VQ
Evaluation B

$C_3H_7NO_2$ (c) 76BER/BOU
Ethyl carbamate; Urethane
Phase Changes
c/liq 321.7 K, $\Delta H = 20900$ J·mol^{-1}
$\Delta S = 64.8$ J·mol^{-1}·K^{-1}
Molecular Weight 75.0871
Wiswesser Line Notation ZVO2
Evaluation A

$C_3H_7NO_2$ (c) 83DEW/DEK
Ethyl carbamate; Urethane
Heat Capacity 300 K, $C_p = 156.43$ J·mol^{-1}·K^{-1}
Temperature range 90 to 330 K.
Phase Changes
c/liq 321.41 K, $\Delta H = 16794$ J·mol^{-1}
$\Delta S = 52.25$ J·mol^{-1}·K^{-1}
Molecular Weight 89.0938
Wiswesser Line Notation ZVO2
Evaluation B(C_p), A(Phase changes).

$C_3H_7NO_3$ (liq) 88LUS/RUB
Isopropyl nitrate
Heat Capacity 298.15 K, $C_p = 191.1$ J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, $S = 263.2$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.81 K, $\Delta H = 10010$ J·mol^{-1}
$\Delta S = 52.43$ J·mol^{-1}·K^{-1}
Molecular Weight 105.0932
Wiswesser Line Notation WNOY1&1
Evaluation A

C_3H_8 (liq) 82VAS
Propane
Heat Capacity 230 K, $C_p = 98.36$ J·mol^{-1}·K^{-1}
Temperature range 90 to 230 K.
C_p given as 2.2305 J·g^{-1}·K^{-1}.
Molecular Weight 44.0962
Wiswesser Line Notation 3H
Evaluation A
Sample purity, 99.95 mol%.

$C_3H_8N_2O$ (c) 87DEL/FER
1,3-Dimethylurea
Phase Changes
c/liq 379.5 K, $\Delta H = 13620$ J·mol^{-1}
$\Delta S = 35.9$ J·mol^{-1}·K^{-1}
Molecular Weight 88.1090
Wiswesser Line Notation 1MVM1
Evaluation A

$C_3H_8N_2O$ (c) 87DEL/FER
1,1-Dimethylurea
Phase Changes
c/liq 454.0 K, $\Delta H = 29610$ J·mol^{-1}
$\Delta S = 65.2$ J·mol^{-1}·K^{-1}
Molecular Weight 88.1090
Wiswesser Line Notation ZVN1&1
Evaluation A

$C_3H_8N_2O$ (c) 87DEL/FER
Ethylurea; Monoethylurea
Phase Changes
c/liq 367.8 K, $\Delta H = 13940$ J·mol^{-1}
$\Delta S = 37.9$ J·mol^{-1}·K^{-1}
Molecular Weight 88.1090
Wiswesser Line Notation ZVM2
Evaluation A

C_3H_8O (liq) 76FOR/BEN2
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298.15 K, $C_p = 144.062$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation A
Data from 76FOR/BEN.

C_3H_8O (liq) 77VES/SVO
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298.15 K, $C_p = 143.78$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 80KAL/JED
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298.216 K, $C_p = 146.34$ J·mol^{-1}·K^{-1}
Temperature range 185 to 300 K.
Unsmoothed experimental datum.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 82VIL/CAS
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298.15 K, $C_p = 146.88$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 84ZEG/SOM
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298.15 K, $C_p = 144.44$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 86KOR/KUK
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298 K, $C_p = 144.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation B

C_3H_8O (liq) 86TAN/TOY
1-Propanol; *n*-Propyl alcohol
Heat Capacity 298.15 K, $C_p = 143.96$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 60.0956
Wiswesser Line Notation Q3
Evaluation A

$C_3H_8O_2$ (liq) 82ZAR
Propylene glycol; 1,2-Propanediol; 1,2-Dihydroxypropane
Heat Capacity 298 K, $C_p = 189.9$ J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 76.0950
Wiswesser Line Notation QY1&1Q
Evaluation B

$C_3H_8O_3$ (liq) 03MAG
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298 K, C_p = 221.9 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.576 cal·g^{-1}·K^{-1}.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation D

$C_3H_8O_3$ (liq) 44YOS
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Phase Changes
c/liq 292 K, ΔH = 18303 J·mol^{-1}
ΔS = 62.7 J·mol^{-1}·K^{-1}
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 82CHE/GE
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 313.15 K, C_p = 229.3 J·mol^{-1}·K^{-1}
Temperature range 20 to 60 K.
C_p given as 2.49 kJ·kg^{-1}·C^{-1} at 40 °C.
C_p at 25 °C estimated from graph to be ca. 2.43 kJ·kg^{-1}·C^{-1} or 223 J·mol^{-1}·K^{-1}.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation B

$C_3H_8O_3$ (liq) 88BAS/NIL
1,2,3-Trihydroxypropane; 1,2,3-Propanetriol; Glycerol
Heat Capacity 298.15 K, C_p = 218.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.0944
Wiswesser Line Notation Q1YQ1Q
Evaluation A

C_3H_9Al 61MCC
Trimethylaluminum
Heat Capacity 298.15 K, C_p = 155.6 J·mol^{-1}·K^{-1}
Temperature Range 10 to 380 K
Entropy 298.15 K, S = 209.4 J·mol^{-1}·K^{-1}
c/liq 288.43 K, ΔH = 8790.6 J·mol^{-1}
ΔS = 30.48 J·mol^{-1}·K^{-1}
Molecular Weight 72.0856
Wiswesser Line Notation 1-AL-1&1
Evaluation A

C_3H_9As (liq) 88NIS/SHE
Trimethyl arsine
Heat Capacity 298.15 K, C_p = 154.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 310 K.
Entropy 298.15 K, S = 251.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 186.60 K, ΔH = 8962 J·mol^{-1}
ΔS = 48.03 J·mol^{-1}·K^{-1}
Molecular Weight 120.0257
Wiswesser Line Notation 1-AS-1&1
Evaluation A

C_3H_9ClSi (liq) 71SAM/KOS
Chlorotrimethylsilane
Heat Capacity 298.15 K, C_p = 187.5 J·mol^{-1}·K^{-1}
Temperature range 12.38 to 303.05 K.
C_p(liq) = 18.19046 + 0.077664T + 309052T^{-2} cal·mol^{-1}·K^{-1}.
Value is calculated from equation.
Deposited in VINITI, No 2501-71, 18 January 1971.
Entropy 298.15 K, S = 275.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 185.1 K, ΔH = 695 J·mol^{-1}
ΔS = 3.75 J·mol^{-1}·K^{-1}
c,I/liq 217.97 K, ΔH = 9682 J·mol^{-1}
ΔS = 44.39 J·mol^{-1}·K^{-1}
Molecular Weight 108.6426
Wiswesser Line Notation G-SI-1&1&1
Evaluation B
T_{Debye} = 115.8 K.

C_3H_9Ga (liq) 88LEB/SMI
Trimethylgallium
Heat Capacity 298.15 K, C_p = 188.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 252.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 244.5 K, ΔH = 333 J·mol^{-1}
ΔS = 1.36 J·mol^{-1}·K^{-1}
c,I/liq 257.81 K, ΔH = 10602 J·mol^{-1}
ΔS = 41.1 J·mol^{-1}·K^{-1}
Molecular Weight 114.8241
Wiswesser Line Notation 1-GA-1&1
Evaluation A

$C_3H_{12}CdCl_4N_2$ (c) 88ABE/CHH
Propyldiammonium cadmium tetrachloride
Heat Capacity 298.15 K, C_p = 275.54 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 298.15 K, S = 351.94 J·mol^{-1}·K^{-1}
Molecular Weight 330.3632
Wiswesser Line Notation Z3Z &GH 2 .CD G2
Evaluation A
Magnetic transition around 50 K.

$C_3H_{12}Cl_4MnN_2$ (c) 85CHH/BOC
Propyldiammonium manganese tetrachloride
Heat Capacity 298.15 K, C_p = 298.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 298.15 K, S = 357.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 307.6 K, ΔH = 710 J·mol^{-1}
ΔS = 2.4 J·mol^{-1}·K^{-1}
DSC study yields ΔH = 725 J·mol^{-1}·K^{-1} at 305 K.
c,II/c,I 336 K, ΔH = 640 J·mol^{-1}
ΔS = 1.90 J·mol^{-1}·K^{-1}
From DSC study.
Molecular Weight 272.8912
Wiswesser Line Notation Z3Z &GH 2 .MN G2
Evaluation A
A magnetic transition is observed in the temperature range 45 to 65 K.

$C_4Br_2Cl_2F_6$ (liq) 88SVO/VES
1,4-Dibromo-2,3-dichlorohexafluorobutane
Heat Capacity 298.16 K, C_p = 298.5 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
C_p (J·mol^{-1}·K^{-1}) = 215.6 + 0.278 (T/K)(298 to 318 K).
Molecular Weight 392.7484
Wiswesser Line Notation FXFEXGFXGFXFFE
Evaluation A

C_4F_8 (liq) 82PON
Freon C318; Octafluorocyclobutane
Heat Capacity 296.41 K, C_p = 222.4 J·mol^{-1}·K^{-1}
Temperature range 240 to 340 K.
Value is unsmoothed experimental datum:
C_p given as 1.112 J·g^{-1}·K^{-1}.
Molecular Weight 200.0312
Wiswesser Line Notation L4TJ AF AF BF BF CF CF DF DF
Evaluation B

C_4F_{10} (liq) 83CAM/DIA
n-Perfluorobutane
Heat Capacity 293 K, C_p = 127.2 J·mol^{-1}·K^{-1}
Calculated value from Sargent, J.W. et al,
Amer. Soc. Test Mater. Spect. Tech. Bull. 346:51, 1964.
Molecular Weight 238.0280
Wiswesser Line Notation FXFFXFFXFFXFFF
Evaluation C

$C_4H_2O_3$ (c) 83DEW/DEK
Maleic anhydride
Heat Capacity 300 K, C_p = 119.9 J·mol^{-1}·K^{-1}
Temperature range 90 to 350 K.
Linearly extrapolated.
Phase Changes
c/liq 325.72 K, ΔH = 13550 J·mol^{-1}
ΔS = 41.6 J·mol^{-1}·K^{-1}
Molecular Weight 98.0580
Wiswesser Line Notation T5VOVJ
Evaluation B(C_p), A(Phase changes).

$C_4H_2O_3$ (c) 83DEW/OFF
Maleic anhydride
Heat Capacity 310 K, C_p = 123.2 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 325.3 K, ΔH = 13600 J·mol^{-1}
ΔS = 41.8 J·mol^{-1}·K^{-1}
Molecular Weight 98.0580
Wiswesser Line Notation T5VOVJ
Evaluation B

$C_4H_2O_4$ (c) 83DEW/OFF
Squaric acid
Heat Capacity 315 K, C_p = 121.6 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c,II/c,I 372.2 K, ΔH = 300 J·mol^{-1}
ΔS = 0.8 J·mol^{-1}·K^{-1}
Molecular Weight 114.0574
Wiswesser Line Notation L4VVJ CQ DQ
Evaluation B

$C_4H_3Cl_3OS$ (liq) 80SHA/LYU
Methyl trichlorothioacrylate
Heat Capacity 298.15 K, C_p = 244.9 J·mol^{-1}·K^{-1}
Temperature range 15 to 330 K.
Entropy 298.15 K, S = 324.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 286.25 K ΔH = 20370 J·mol^{-1}
ΔS = 71.2 J·mol^{-1}·K^{-1}
Molecular Weight 205.4861
Wiswesser Line Notation GYGUYGVS1
Evaluation A

C_4H_3Cu (c) 82BYK/LEB
Copper vinylacetylenide
Heat Capacity 298.15 K, C_p = 109.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 132.6 J·mol^{-1}·K^{-1}
Molecular Weight 114.6137
Wiswesser Line Notation -CU-1U12U1
Evaluation A

$C_4H_3F_5O_3$ (liq) 84GOL/KOL
α-(Trifluoromethoxy)-α,α-difluoromethyl acetate
Phase Changes
c/liq 167.4 K, ΔH = 8510 J·mol^{-1}
ΔS = 50.8 J·mol^{-1}·K^{-1}
Molecular Weight 194.0579
Wiswesser Line Notation FXFFOXFFVO1
Evaluation A

$C_4H_4KNaO_6{\cdot}4H_2O$ (c) 38HIC/HOO
Sodium potassium tartrate tetrahydrate;
Rochelle salt
Heat Capacity 300 K, C_p = 389.1 J·mol^{-1}·K^{-1}
Temperature range 15 to 340 K.
Phase Changes
c,II/c,I 328.78 K, ΔH = 42752 J·mol^{-1}
ΔS = 130.0 J·mol^{-1}·K^{-1}
Molecular Weight 282.2209
Wiswesser Line Notation OVYQYQVO .K .NA &QH4
Evaluation B

$C_4H_4N_2$ (c) 87RAI/SIN
Succinonitrile; 1,4-Butanedinitrile
Phase Changes
c/liq 334 K, ΔH = 3704 J·mol^{-1}
ΔS = 11.1 J·mol^{-1}·K^{-1}
Molecular Weight 80.0890
Wiswesser Line Notation NC2CN
Evaluation B

$C_4H_4N_2O_3$ (c) 85KOS/ISM
Barbituric acid
Heat Capacity 298.15 K, C_p = 141.1 J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.15 K, S = 157.6 J·mol^{-1}·K^{-1}
Extrapolated below 90 K.
Molecular Weight 128.0872
Wiswesser Line Notation T6VMVMV FHJ
Evaluation B(C_p), C(S)

$C_4H_4O_4$ (c,II) 77LEB/EVS
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p = 133.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S = 157.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH = 1840 J·mol^{-1}
ΔS = 5.90 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH = 14800 J·mol^{-1}
ΔS = 41.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A

$C_4H_4O_4$ (c,II) 78EVS/BEL
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p = 133.3 J·mol^{-1}·K^{-1}
Temperature range 8 to 400 K.
Entropy 298.15 K, S = 157.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH = 1810 J·mol^{-1}
ΔS = 5.80 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH = 14800 J·mol^{-1}
ΔS = 41.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A
See also 77EVS/BEL.

$C_4H_4O_4$ (c,II) 78LEB/YEV
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p = 133.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S = 157.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH = 1810 J·mol^{-1}
ΔS = 5.80 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH = 14800 J·mol^{-1}
ΔS = 41.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A
Data also given for metastable crystalline phase, c,I′ at 298.15 K: C_p = 137.0 J·mol^{-1}·K^{-1} and $S_T°$ = 163.1 J·mol^{-1}·K^{-1}.

$C_4H_4O_4$ (c,II) 88LEB/KUL
Glycolide; 1,4-Dioxane-2,5-dione
Heat Capacity 298.15 K, C_p = 133.28 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 400 K.
Entropy 298.15 K, S = 157.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH = 1840.0 J·mol^{-1}
ΔS = 5.90 J·mol^{-1}·K^{-1}
c,I/liq 356.2 K, ΔH = 14800 J·mol^{-1}
ΔS = 41.49 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV DOVTJ
Evaluation A

$C_4H_4O_4$ (c) 82LEB/KUL
Ethylene oxalate
Heat Capacity 298.15 K, C_p = 141.9 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 149.7 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV VOTJ
Evaluation A

$C_4H_4O_4$ (c) 82LEB/KUL2
Ethylene oxalate
Heat Capacity 298.15 K, C_p = 141.9 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 158.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 415 K, ΔH = 13400 J·mol^{-1}
ΔS = 32.29 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation T6OV VOTJ
Evaluation A

$(C_4H_4O_4)_n$ (c) 77LEB/EVS
Polyglycolide
Heat Capacity 298.15 K, C_p = 130.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S = 150.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 501 K, ΔH = 23500 J·mol^{-1}
ΔS = 47 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation /*V1OV1O*/
Evaluation A
T(glass) = 318 K.

$(C_4H_4O_4)_n$ (gls) 78LEB/YEV
Polyglycolide
Heat Capacity 298.15 K, C_p = 136.7 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 550 K.
Entropy 298.15 K, S = 151.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 501 K, ΔH = 23500 J·mol^{-1}
ΔS = 47 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation /*V1OV1O*/
Evaluation A
T(glass) = 318 K.

$(C_4H_4O_4)_n$ (gls) 82LEB/KUL2
Polyethylene oxalate
Heat Capacity 298.15 K, C_p = 129.1 J·mol^{-1}·K^{-1}
Temperature range 8 to 360 K.
Entropy 298.15 K, S = 163.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.0732
Wiswesser Line Notation /*VVO2O*/
Evaluation A

C_4H_4S (c) 82AND/DWO
Thiophene
Heat Capacity
Temperature range 50 to 200 K.
Data graphically only in the region of the phase transitions.
Phase Changes
c,V/c,IV 111.3 K
c,IV/c,III 136.8 K
c,III/c,II 170.5 K
c,II/c,I 174.5 K
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation A

C_4H_4S (c) 84FIG/SZW
Thiophene
Heat Capacity
Temperature range 14 to 300 K. Data given graphically only.
Phase Changes
c,V'/c,IV' 90.76 K
Metastable transition.
c,IV'/c,III' 139.2 K
Metastable transition.
c,V/c,IV 112.35 K
c,IV/c,III 138.5 K
c,III/c,II 170.70 K
c,II/c,I 175.03 K
c,I/liq 235.03 K
Molecular Weight 84.1356
Wiswesser Line Notation T5SJ
Evaluation A

C_4H_5NO (liq) 79DZH/KAR
β-Cyanopropionaldehyde
Heat Capacity 300 K, C_p = 195.9 J·mol^{-1}·K^{-1}
Temperature range 55 to 300 K.
Phase Changes
c,II/c,I 140 K
c,I/liq 230 K
Molecular Weight 83.0896
Wiswesser Line Notation VH2CN
Evaluation C

C_4H_5NO (liq) 81MUS/GAN
α-Cyanopropionaldehyde
Heat Capacity 300 K, C_p = 169.5 J·mol^{-1}·K^{-1}
Temperature range 220 to 370 K.
C_p given as 2040 J·kg^{-1}·K^{-1}.
Molecular Weight 83.0896
Wiswesser Line Notation VHY1&CN
Evaluation C

$(C_4H_6)_n$ (liq) 86GRE/AYC
cis-1,4-Polybutadiene
Heat Capacity 298.2 K, C_p = 105.7 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K
Entropy 298.2 K, S = 126.68 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 284 K
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/ -C
Evaluation A

$(C_4H_6)_n$ (c) 86GRE/AYC
trans-1,4-Polybutadiene
Heat Capacity 298.2 K, C_p = 87.59 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K
Entropy 298.2 K, S = 91.23 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 356 K ΔH = 7980 J·mol^{-1}
ΔS = 21.9 J·mol^{-1}·K^{-1}
Fully ordered/conformationally disordered transition
c,I/liq 437 K
Molecular Weight 54.0914
Wiswesser Line Notation /*2U2*/ -T
Evaluation A

$C_4H_6N_2O_2$ (c) 82LEB/KUL
2,5-Dioxopiperazine
Heat Capacity 298.15 K, C_p = 134.0 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 145.5 J·mol^{-1}·K^{-1}
Molecular Weight 114.1036
Wiswesser Line Notation T6MV DMVTJ
Evaluation A

$C_4H_6O \cdot 17H_2O$ (liq) 85HAN
2,5-Dihydrofuran clathrate hydrate
Heat Capacity 260 K, C_p = 726 J·mol^{-1}·K^{-1}
Temperature range 95 to 260 K.
Phase Changes
c,I/liq 272.0 K, ΔH = 92900 J·mol^{-1}
ΔS = 341.5 J·mol^{-1}·K^{-1}
Molecular Weight 70.0908
Wiswesser Line Notation T5O BH EHJ &QH 17
Evaluation A
Actual composition is a mixed hydrate:
0.978 DHF– 0.022 THF– 17 H_2O.

C_4H_6O (liq) 88BAG/GUR
2-Butenal; Crotonaldehyde
Heat Capacity 298.35 K, C_p = 148.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 70.0908
Wiswesser Line Notation VH1U2
Evaluation B

$C_4H_6O_2$ (liq) 84VAS/PET
Methyl propenoate; Methyl acrylate
Heat Capacity 300 K, C_p = 158.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S = 239.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 196.21 K
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation A

$C_4H_6O_2$ (liq) 85KAR/ABD2
Methyl propenoate; Methyl acrylate
Phase Changes
c/liq 197.5 K, ΔH = 9729 J·mol^{-1}
ΔS = 49.26 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation 1U1VO1
Evaluation A

$C_4H_6O_2$ (liq) 83LEB/YEV
τ-Butyrolactone
Heat Capacity 298.15 K, C_p = 141.3 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S = 197.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.78 K, ΔH = 9570 J·mol^{-1}
ΔS = 41.56 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation T5OVTJ
Evaluation A

$C_4H_6O_2$ (liq) 84VAS/PET
Methacrylic acid; α-Methyl acrylic acid
Heat Capacity 300 K, C_p = 161.1 J·mol^{-1}·K^{-1}
Temperature range 25 to 300 K.
Entropy 300 K, S = 186.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 289.36 K
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation A

$C_4H_6O_2$ (liq) 85KAR/ABD
Methacrylic acid; α-Methyl acrylic acid
Heat Capacity 298.15 K, C_p = 159.7 J·mol^{-1}·K^{-1}
Temperature range 287 to 350 K. Equation only.
C_p (J·kg^{-1}·K^{-1}) = −551.8 + 8.0712 T.
C_p data calculated from equation.
Phase Changes
c/liq 287.5 K
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation B

$C_4H_6O_2$ (liq) 85KAR/ABD2
Methacrylic acid; α-Methyl acrylic acid
Phase Changes
c/liq 287.5 K, ΔH = 8062.5 J·mol^{-1}
ΔS = 28.04 J·mol^{-1}·K^{-1}
Molecular Weight 86.0902
Wiswesser Line Notation QVY1&U1
Evaluation A

$(C_4H_6O_2)_n$ (c) 67PAV/RAB
Polymethacrylic acid
Heat Capacity 298 K, C_p = 92.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 463 K.
C_p = 0.233 + 9.00×10^{-4}T cal·g·°C (20 to 130 °C).
Value calculated from equation.
Molecular Weight 86.0902
Wiswesser Line Notation /*1X*1&VQ/
Evaluation B
T(glass) = 433 K.

$C_4H_6O_3$ (liq) 76VAS/KOR
Propylene carbonate
Heat Capacity 298.15 K, C_p = 167.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 415 K.
Entropy 298.15 K, S = 218.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 224.85 K, ΔH = 9617 J·mol^{-1}
ΔS = 42.8 J·mol^{-1}·K^{-1}
Molecular Weight 102.0896
Wiswesser Line Notation T5OVOTJ D1
Evaluation A

$C_4H_6O_3$ (liq) 84VAS/PET
Propylene carbonate
Heat Capacity 298.15 K, C_p = 167.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 415 K.
Entropy 298.15 K, S = 218.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 224.85 K, ΔH = 9620 J·mol^{-1}
ΔS = 42.8 J·mol^{-1}·K^{-1}
Molecular Weight 102.0896
Wiswesser Line Notation T5OVOTJ D1
Evaluation A

$C_4H_6O_4Mg$ (gls) 71ONO/KIM
Magnesium acetate
Heat Capacity 310.02 K, C_p = 20.452 J·mol^{-1}·K^{-1}
Temperature range 310 to 500 K.
Unsmoothed experimental datum.
Data also given for crystalline state from 348 to 501 K.
Molecular Weight 142.3942
Wiswesser Line Notation OV1 2 .MG
Evaluation B
T(glass) = 470 K.

$C_4H_6O_4Mg·4H_2O$ (c) 84MEI/GRO
Magnesium diethanoate tetrahydrate;
Magnesium diacetate tetrahydrate
Heat Capacity 298.15 K, C_p = 321.0 J·mol^{-1}·K^{-1}
Temperature range 270 to 400 K.
Phase Changes
c/aq 336 K, ΔH = 35800 J·mol^{-1}
ΔS = 106.5 J·mol^{-1}·K^{-1}
Transition of tetrahydrate to less hydrated salt, presumably the monohydrate.
Molecular Weight 214.4548
Wiswesser Line Notation OV2 2 .MG &QH 4
Evaluation B

$C_4H_6O_4Zn$ (c) 84SPI/PRO
Zinc acetate
Heat Capacity 298 K, C_p = 153.6 J·mol^{-1}·K^{-1}
Temperature range 243 to 293 K.
Value calculated from equation:
C_p(kJ·mol^{-1}·K^{-1}) = 3.44×10^{-2} + 4×10^{-4}T(K).
Molecular Weight 183.4690
Wiswesser Line Notation OV1 2 .ZN
Evaluation C

$C_4H_6O_4Zn·2H_2O$ (c) 84SPI/PRO
Zinc acetate dihydrate
Heat Capacity 298 K, C_p = 212.8 J·mol^{-1}·K^{-1}
Temperature range 243 to 293 K.
Value calculated from equation:
C_p(kJ·mol^{-1}·K^{-1}) = 3.40×10^{-2} + 6×10^{-4}T(K).
Molecular Weight 219.4994
Wiswesser Line Notation OV1 2 .ZN &QH 2
Evaluation C

$C_4H_7KO_2$ (c) 87FRA/NGE
Potassium butyrate
Heat Capacity 298.15 K, C_p = 157.97 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S = 211.52 J·mol^{-1}·K^{-1}
Phase Changes
c,VII/c,VI 123.85 K, ΔH = 409 J·mol^{-1}
ΔS = 3.33 J·mol^{-1}·K^{-1}
c,VI/c,VB 142.3 K, ΔH = 269 J·mol^{-1}
ΔS = 1.88 J·mol^{-1}·K^{-1}
Bifurcated transitions.
c,VB/c,V*A* 250 K
Diffuse anomaly in heat capacity curve.
c,V/c,IV 461.4 K
c,IV/c,III 467.2 K
c,III/c,II 541 K
c,II/c,I 562.2 K
c,I/liq 626.1 K
Solid-liquid crystal.
Molecular Weight 126.1964
Wiswesser Line Notation OV3 .KA
Evaluation A
Liquid crystal-isotropic liquid transition at 677.3 K.

$C_4H_7KO_2$ (c) 84FRA/WES2
Potassium 2-methylpropanoate
Heat Capacity 298.15 K, C_p = 166.95 J·mol^{-1}·K^{-1}
Temperature range 8 to 350 K.
Entropy 298.15 K, S = 192.40 J·mol^{-1}·K^{-1}
Molecular Weight 126.1964
Wiswesser Line Notation OVY1&1 .KA
Evaluation A

$C_4H_7LiO_2$ (c) 86NGE/WES
Lithium butyrate
Heat Capacity 298.15 K, C_p = 153.40 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 173.36 J·mol^{-1}·K^{-1}
Molecular Weight 94.0391
Wiswesser Line Notation OV3 .LI
Evaluation A

C_4H_7NO (liq) 62KOL/PAU
α-Pyrrolidone
Heat Capacity 300.00 K, C_p = 169.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 310.00 K, S = 189.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 299.082 K, ΔH = 13920 J·mol^{-1}
ΔS = 46.5 J·mol^{-1}·K^{-1}
Molecular Weight 85.1033
Wiswesser Line Notation T5MVTJ
Evaluation B

$C_4H_7O_2Tl$ (c) 76MEI/SEY
Thallium butyrate
Phase Changes
c,I/liq 459 K, ΔH = 6694 J·mol^{-1}
ΔS = 14.2 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 291.4681
Wiswesser Line Notation OV3 .TL
Evaluation B

$C_4H_7O_2Tl$ (c) 84FER/LOP
Thallium butyrate
Heat Capacity 320 K, C_p = 175 J·mol^{-1}·K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,I/liq 456.7 K, ΔH = 7691 J·mol^{-1}
ΔS = 16.9 J·mol^{-1}·K^{-1}
Molecular Weight 291.4681
Wiswesser Line Notation OV3 .TL
Evaluation A

C_4H_8 (liq) 71RAB/LEB
2-Methylpropene; Isobutene
Heat Capacity 266.26 K, C_p = 121.3 J·mol^{-1}·K^{-1}
Temperature range 90 to 266 K.
Phase Changes
c/liq 132.38 K
liq/g 266.26 K
Molecular Weight 56.1072
Wiswesser Line Notation 1Y1&U1
Evaluation B

C_4H_8 (liq) 83CHA/HAL
cis-2-Butene
Heat Capacity 298.15 K, C_p = 127 J·mol^{-1}·K^{-1}
Temperature range 5 to 367 K.
Entropy 298.15 K, S = 220 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 134.26 K, ΔH = 7309 J·mol^{-1}
ΔS = 54.4 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 −C
Evaluation A
A reevaluation of the original measured data from: 36TOD/PAR, 44SCO/FER, 52SCH/SAG.

C_4H_8 (liq) 83CHA/HAL
trans-2-Butene
Heat Capacity 280 K, C_p = 124.4 J·mol^{-1}·K^{-1}
Temperature range 14 to 271 K.
Entropy 280 K, S = 163.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 167.62 K, ΔH = 9757 J·mol^{-1}
ΔS = 58.2 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation 2U2 −T
Evaluation A
A reevaluation of the original measured data from: 36TOD/PAR, 45GUT/PIT.

C_4H_8 (liq) 49SCH/SAG
1-Butene
Heat Capacity 294 K, C_p = 128.6 J·mol^{-1}·K^{-1}
Temperature range 294 to 378 K.
C_p given as 0.548 Btu(lb)$^{-1}$(°R)$^{-1}$ at 70°F at bubble point.
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation B

C_4H_8 (liq) 83CHA/HAL
1-Butene
Heat Capacity 298.15 K, C_p = 118 J·mol^{-1}·K^{-1}
Temperature range 12 to 360 K.
Entropy 298.15 K, S = 227.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 87.82 K, ΔH = 3848 J·mol^{-1}
ΔS = 43.8 J·mol^{-1}·K^{-1}
Molecular Weight 56.1072
Wiswesser Line Notation 3U1
Evaluation A
A reevaluation of the original measured data from: 46AST/FIN, 49SCH/SAG, 36TOD/PAR.

$(C_4H_8)_n$ (c) 71RAB/LEB
Polyisobutylene
Heat Capacity 300 K, C_p = 109.7 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Molecular Weight 56.1072
Wiswesser Line Notation /*1X*1&1/
Evaluation A

$C_4H_8Cl_2$ (liq) 85LAI/WIL
1,4-Dichlorobutane
Heat Capacity 298.15 K, C_p = 183.59 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 127.0132
Wiswesser Line Notation G4G
Evaluation A

$C_4H_8N_8O_8$ (c,α) 70LIC
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(α); Octogen(α); HMX
Heat Capacity 298 K, C_p = 307 J·mol^{-1}·K^{-1}
Temperature range 203 to 523 K. α-Phase.
C_p = 0.0991 + 5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C).
Phase Changes
c,II/c,I 193–201 K, ΔH = 7398 J·mol^{-1}
α-δ Transition.
Data also given for the following transitions:
β-δ; T = 167 to 183 °C; ΔH = 9801 J·mol^{-1}.
τ-δ; T = 175 to 182 °C; ΔH = 2788 J·mol^{-1}.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation B
Data also given for the following polymorphic forms:
β-HMX; C_p(298 K) = 301 J·mol^{-1}·K^{-1};
C_p = 0.0935 + 5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C);
τ-HMX; C_p(298 K) = 328 J·mol^{-1}·K^{-1};
C_p = 0.1159 + 5×10^{-4}T cal·K^{-1}·g^{-1} (−70 to 250 °C);
δ-HMX; C_p(298 K) = 387 J·mol^{-1}·K^{-1};
C_p = 0.1642 + 5×10^{-4}T cal·K^{-1}·g^{-1} (-70 to 250 °C).

$C_4H_8N_8O_8$ (c,β) 83KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(β); Octogen(β); HMX
Heat Capacity 315 K, C_p = 321.0 J·mol^{-1}·K^{-1}
Temperature range 294 to 486 K. β-phase, powdered blend.
C_p given as 1.084 J·g^{-1}·K^{-1}.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation B

$C_4H_8N_8O_8$ (c) 83KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine; Octogen; HMX
Heat Capacity 298 K, C_p = 293 J·mol^{-1}·K^{-1}
Temperature range 294 to 486 K.
Graphical extrapolation of data to 298 K; powdered blend.
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

$C_4H_8N_8O_8$ (c,β) 84KOS/SHO
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(β); Octogen(β); HMX
Heat Capacity 298 K, C_p = 297 J·mol^{-1}·K^{-1}
Temperature range 294 to 486 K.
Graphical extrapolation of data to 298 K; single crystals, beta phase.
Phase Changes
c,II/c,I 453 K
(c,beta/c,delta)
Molecular Weight 296.1560
Wiswesser Line Notation T8N CN EN GNTJ ANW CNW ENW GNW
Evaluation C

C_4H_8O (liq) 88BAG/GUR
2-Methoxy-1-propene
Heat Capacity 301.50 K, C_p = 162.2 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 72.1066
Wiswesser Line Notation 1YO1U1
Evaluation B

C_4H_8O (liq) 84GRO/BEN
Butanone; Methyl ethyl ketone
Heat Capacity 298.15 K, C_p = 157.91 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 86RED
Butanone; Methyl ethyl ketone
Heat Capacity 303.15 K, C_p = 162.2 J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 72.1066
Wiswesser Line Notation 2V1
Evaluation B

C_4H_8O (liq) 77LEB/LIT2
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 K, C_p = 123.9 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S = 203.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 164.76 K, ΔH = 8540 J·mol^{-1}
ΔS = 51.83 J·mol^{-1}·K^{-1}
liq/g 338.9 K
Molecular Weight 72.1066
Wiswesser Line Notation T5OTJ
Evaluation A

C_4H_8O (liq) 79LEB/LIT
Tetrahydrofuran; Oxolane
Heat Capacity 298.15 *K*
Temperature range 8 to 322 K
Entropy 298.15 K $S = 203.9$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 164.76 K $\Delta H = 8540$ *J* mol^{-1}
$\Delta S = 51.83$ J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation T5OTU
Evaluation A

$C_4H_8O \cdot 17H_2O$ (liq) 85HAN
Tetrahydrofuran clathrate hydrate
Heat Capacity
Temperature range 95 to 260 K.
Phase Changes
c/liq 277.3 K, $\Delta H = 99100$ J·mol^{-1}
$\Delta S = 357.4$ J·mol^{-1}·K^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O \cdot 17H_2O$.

$C_4H_8O \cdot 17H_2O$ (c) 82LEA/MUR
Tetrahydrofuran clathrate hydrate
Heat Capacity
Temperature range 120 to 260 K.
Data given graphically.
Phase Changes
c/liq 277.4 K, $\Delta H = 98000$ J·mol^{-1}
$\Delta S = 353.2$ J·mol^{-1}·K^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O \cdot 16.9H_2O$

$C_4H_8O \cdot 17H_2O$ (liq) 88YAM/OGU
Tetrahydrofuran clathrate hydrate
Heat Capacity 298.15 K, $C_p = 1523.2$ J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, $S = 1298.7$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 85 K
Glass transition.
c/liq 277.4 K, $\Delta H = 96980$ J·mol^{-1}
$\Delta S = 349.6$ J·mol^{-1}·K^{-1}
Molecular Weight 378.3650
Wiswesser Line Notation T5OTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O \cdot 16.64H_2O$.

$(C_4H_8O)_n$ (c) 77LEB/LIT
Polytetrahydrofuran
Phase Changes
c,II/c,I 186 K
Glass point.
c/liq 316 K, $\Delta H = 11000$ J·mol^{-1}
$\Delta S = 34.8$ J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation /*O4*/
Evaluation A

$(C_4H_8O)_n$ (c) 77LEB/LIT2
Polytetrahydrofuran
Heat Capacity 200 K, $C_p = 81.30$ J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Transition region at 298.15 K.
Entropy 200 K, $S = 83.06$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 316 K, $\Delta H = 11000$ J·mol^{-1}
$\Delta S = 34.8$ J·mol^{-1}·K^{-1}
Molecular Weight 72.1066
Wiswesser Line Notation /*O4*/
Evaluation A
T(glass) = 186 K.

$C_4H_8O_2$ (liq) 86JIM/ROM
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.15 K, $C_p = 169.30$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2OV1
Evaluation B

$C_4H_8O_2$ (liq) 87ZAB/HYN
Ethyl acetate; Ethyl ethanoate
Heat Capacity 298.32 K, $C_p = 170.59$ J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 20V1
Evaluation B

$C_4H_8O_2$ (liq) 84GUS/SHU
Methyl propionate; Methyl propanoate
Heat Capacity 298.38 K, $C_p = 175.9$ J·mol^{-1}·K^{-1}
Temperature range 205 to 348 K.
Unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation C

$C_4H_8O_2$ (liq) 86JIM/ROM
Methyl propionate; Methyl propanoate
Heat Capacity 298.15 K, $C_p = 172.74$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 87ZAB/HYN
Methyl propionate; Methyl propanoate
Heat Capacity 301.45 K, $C_p = 174.60$ J·mol^{-1}·K^{-1}
Temperature range 296 to 342 K.
Unsmoothed experimental datum.
Molecular Weight 88.1060
Wiswesser Line Notation 2VO1
Evaluation B

$C_4H_8O_2$ (liq) 86JIM/ROM
Propyl methanoate; Propyl formate
Heat Capacity 298.15 K, $C_p = 171.42$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation 30VH
Evaluation B

$C_4H_8O_2$ (liq) 82BIR/SIK
Isobutyric acid; 2-Methylpropanoic acid
Heat Capacity 298.15 K, C_p = 181.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K.
Equation only.
C_p = 130.1 − 0.08156 T + 0.0008541 T^2 J·mol^{-1}·K^{-1}.
Molecular Weight 88.1060
Wiswesser Line Notation QVY1&1
Evaluation C

$C_4H_8O_2$·17H_2O (liq) 85HAN
1,3-Dioxane clathrate hydrate
Heat Capacity 250 K, C_p = 745 J·mol^{-1}·K^{-1}
Temperature range 95 to 250 K.
Phase Changes
c,I/liq 269.6 K, ΔH = 89900 J·mol^{-1}
ΔS = 333.5 J·mol^{-1}·K^{-1}
Molecular Weight 394.3644
Wiswesser Line Notation T6O COTJ &QH 17
Evaluation A
Actual formula: $C_4H_8O_2$·17H_2O.

$C_4H_8O_2$ (liq) 69SUB/KHA
1,4-Dioxane
Heat Capacity 298 K, C_p = 147.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation C

$C_4H_8O_2$ (liq) 79MUR/SUB
1,4-Dioxane
Heat Capacity 298 K, C_p = 149.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_2$ (liq) 84GRO/ING
1,4-Dioxane
Heat Capacity 298.15 K, C_p = 150.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1060
Wiswesser Line Notation T6O DOTJ
Evaluation B

$C_4H_8O_3$ (liq) 83SAN/CIO
Ethylene glycol acetate
Heat Capacity 298.15 K C_p = 203 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K
C_p° (kJ·kg^{-1}·K^{-1}) = 0.042568T - 10.686
Molecular Weight 101.0817
Wiswesser Line Notation Q2OV1
Evaluation D

$C_4H_8S_2$ (c) 83DEW/OFF
1,3-Dithiane
Heat Capacity 300 K, C_p = 113.9 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c,II/c,I 316.4 K, ΔH = 800 J·mol^{-1}
ΔS = 2.5 J·mol^{-1}·K^{-1}
c,I/liq 327.2 K, ΔH = 14400 J·mol^{-1}
ΔS = 44.0 J·mol^{-1}·K^{-1}
Molecular Weight 120.2272
Wiswesser Line Notation T6S CSTJ
Evaluation B

$C_4H_8S_2$ (c) 83DEW/OFF
1,4-Dithiane
Heat Capacity 300 K, C_p = 129.8 J·mol^{-1}·K^{-1}
Temperature range 300 to 450 K.
Phase Changes
c/liq 384.6 K, ΔH = 21600 J·mol^{-1}
ΔS = 56.2 J·mol^{-1}·K^{-1}
Molecular Weight 120.2272
Wiswesser Line Notation T6S DSTJ
Evaluation B

C_4H_9Cl (liq) 85LAI/WIL
1-Chlorobutane; n-Butyl chloride
Heat Capacity 298.15 K, C_p = 159.64 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.5681
Wiswesser Line Notation G4
Evaluation A

C_4H_9NO (c) 80LYA
Morpholine; Tetrahydro-1,4-isoxazine; Diethyleneimide oxide
Heat Capacity 298.15 K, C_p = 164.8 J·mol^{-1}·K^{-1}
Temperature range 293 to 353 K.
Data given graphically.
C_p value calculated from equation:
C_p(J·g^{-1}·K^{-1}) = 1.785 + 0.00427 T(°C).
Molecular Weight 87.1212
Wiswesser Line Notation T6M DOTJ
Evaluation C

C_4H_9NO (c) 89ABB/JIM
2-Methylpropanamide
Heat Capacity 298.15 K, C_p = 148.1 J·mol^{-1}·K^{-1}
One temperature; C_p given as 1.70 J·g^{-1}·K^{-1}.
Phase Changes
c/g 298.15 K, ΔH = 86000 J·mol^{-1}
ΔS = 288.4 J·mol^{-1}·K^{-1}
Molecular Weight 87.1212
Wiswesser Line Notation ZVY1&1
Evaluation A

$C_4H_9NO_2$ (c) 83SKO/SAB
4-Aminobutanoic acid; τ-Aminobutyric acid
Heat Capacity 298 K, C_p = 133.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 103.1206
Wiswesser Line Notation Z3VQ
Evaluation B

$C_4H_9NO_2$ (c) 84GRU/BOU
α-Aminobutyric acid (L); 2-Aminobutanoic acid (L)
Phase Changes
c,II/c,I 356 K, ΔH = 530 J·mol^{-1}
ΔS = 1.49 J·mol^{-1}·K^{-1}
Molecular Weight 103.1206
Wiswesser Line Notation ZY2&QV -L
Evaluation B

$C_4H_{10}Hg$ (liq) 78BUR/KAM
Diethyl mercury
Heat Capacity 298.15 K, C_p = 182.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Phase Changes
c/liq 181.45 K, ΔH = 10500 J·mol^{-1}
ΔS = 57.87 J·mol^{-1}·K^{-1}
Molecular Weight 258.7130
Wiswesser Line Notation 2-HG-2
Evaluation A

$C_4H_{10}N_2$ (liq) 88BOB/KAM
Piperazine
Heat Capacity 413 K, C_p = 237 J·mol^{-1}·K^{-1}
Temperature range 413 to 473 K.
Molecular Weight 86.1364
Wiswesser Line Notation T6M DMTU
Evaluation D

$C_4H_{10}N_2O$ (c) 87DEL/FER
1,1,3-Trimethylurea
Phase Changes
c/liq 344.4 K, ΔH = 14300 J·mol^{-1}
ΔS = 41.5 J·mol^{-1}·K^{-1}
Molecular Weight 102.1358
Wiswesser Line Notation 1MVN1&1
Evaluation A

$C_4H_{10}N_2O$ (c) 87DEL/FER
Isopropylurea; Monoisopropylurea
Phase Changes
c,II/c,I 375.5 K, ΔH = 2310 J·mol^{-1}
c/liq 427.4 K, ΔH = 17400 J·mol^{-1}
ΔS = 40.7 J·mol^{-1}·K^{-1}
Molecular Weight 102.1358
Wiswesser Line Notation ZVMY1&1
Evaluation A

$C_4H_{10}N_2O$ (c) 87DEL/FER
Propylurea; Monopropylurea
Phase Changes
c/liq 381.0 K, ΔH = 14630 J·mol^{-1}
ΔS = 38.4 J·mol^{-1}·K^{-1}
Molecular Weight 102.1358
Wiswesser Line Notation ZVM3
Evaluation A

$C_4H_{10}O$ (liq) 75FEN/HAR
2-Oxapentane; Methyl *n*-propyl ether
Heat Capacity 298.15 K, C_p = 165.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation 3O1
Evaluation B

$C_4H_{10}O$ (liq) 78RYB/EME
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 303.15 K, C_p = 185.6 J·mol^{-1}·K^{-1}
Temperature range 293.15 to 353.15 K.
C_p given as 2504 J·kg^{-1}·K^{-1}.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation C

$C_4H_{10}O$ (liq) 88OKA/OGA
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 298.15 K, C_p = 181.05 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation B

$C_4H_{10}O$ (liq) 88PIE/SOM
Isobutyl alcohol; 2-Methyl-1-propanol
Heat Capacity 298.15 K, C_p = 182.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q1Y1&1
Evaluation B

$C_4H_{10}O$ (liq) 84ZEG/SOM
1-Butanol; *n*-Butyl alcohol
Heat Capacity 298.15 K, C_p = 177.08 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86GAT/WOO
1-Butanol; *n*-Butyl alcohol
Heat Capacity 298.15 K, C_p = 176.67 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 368.15 K.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation C

$C_4H_{10}O$ (liq) 86KOR/KUK
1-Butanol; *n*-Butyl alcohol
Heat Capacity 298 K, C_p = 177.7 J·mol^{-1}·K^{-1}
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation B

$C_4H_{10}O$ (liq) 86TAN/TOY
1-Butanol; *n*-Butyl alcohol
Heat Capacity 298.15 K, C_p = 176.69 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation Q4
Evaluation A

$C_4H_{10}O$ (liq) 76SKO/SUU
tert-Butyl alchohol; 2-Methyl-2-propanol
Heat Capacity 298.15 K, C_p = 218.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation A

$C_4H_{10}O$ (liq) 88OKA/OGA
tert-Butyl alcohol; 2-Methyl-2-propanol
Heat Capacity 299.15 K, C_p = 221.88 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QX1&1&1
Evaluation B

$C_4H_{10}O$ (liq) 88OKA/OGA
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p = 198.03 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation B

$C_4H_{10}O$ (liq) 88PIE/SOM
2-Butanol; sec-Butyl alcohol
Heat Capacity 298.15 K, C_p = 196.67 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 74.1224
Wiswesser Line Notation QY2&1
Evaluation B

$(C_4H_{10}OSi)_n$ (liq) 82KUL/LEB
Poly(diethylsiloxane)
Heat Capacity 298.15 K, C_p = 165.5 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S = 215.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 203 K, ΔH = 2070 J·mol^{-1}
ΔS = 10.2 J·mol^{-1}·K^{-1}
Degree of crystallinity = 72%.
c/liq 295 K, ΔH = 2876 J·mol^{-1}
ΔS = 9.75 J·mol^{-1}·K^{-1}
Degree of crystallinity = 100%.
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A
T(glass) = 130 K

$(C_4H_{10}OSi)_n$ (liq) 84LEB/KUL
Poly(diethylsiloxane)
Heat Capacity 298.15 K, C_p = 165.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S = 215.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 203 K, ΔH = 2070 J·mol^{-1}
ΔS = 10.2 J·mol^{-1}·K^{-1}
Degree of crystallinity = 72%.
c,I/liq 295 K, ΔH = 2860 J·mol^{-1}
ΔS = 9.75 J·mol^{-1}·K^{-1}
Degree of crystallinity = 100%.
Molecular Weight 102.2079
Wiswesser Line Notation /*-SI-2&2&O*/
Evaluation A
T(glass) = 130 K

$C_4H_{10}O_2$ (liq) 84VAS/PET
1,4-Butanediol; 1,4-Dihydroxybutane
Heat Capacity 298.15 K, C_p = 200.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 450 K.
Entropy 298.15 K, S = 223.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 293.58 K, ΔH = 18700 J·mol^{-1}
ΔS = 63.7 J·mol^{-1}·K^{-1}
Molecular Weight 90.1218
Wiswesser Line Notation Q4Q
Evaluation A

$C_4H_{10}O_2Se$ (liq) 83GEI/GUS
β-Selenodiglycol
Heat Capacity 298.15 K, C_p = 349.9 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S = 358.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 154.0 K, ΔH = 110 J·mol^{-1}
ΔS = 0.7 J·mol^{-1}·K^{-1}
Glassy (solid) to liquid.
Molecular Weight 169.0818
Wiswesser Line Notation Q2-SE-2Q
Evaluation A

$C_4H_{10}O_3$ (liq) 82ZAR
Diethylene glycol; 1,5-Dihydroxy-3-oxapentane
Heat Capacity 298 K, C_p = 243.9 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 106.1212
Wiswesser Line Notation Q2O2Q
Evaluation B

$C_4H_{10}O_3$ (c) 89ZHA/YAN
1,1,1-Trihydroxymethylpropane
Heat Capacity 301.29 K 213.79 J·mol^{-1}·K^{-1}
Temperature range 270 to 354 K. Value is unsmoothed experimental datum.
Phase Changes
c/liq 333.40 K ΔH = 21450 J·mol^{-1}
ΔS = 64.3 J·mol^{-1}·K^{-1}
Molecular Weight 106.1212
Wiswesser Line Notation QXQQY1&1
Evaluation A

$C_4H_{10}S$ (liq) 82TUT/GAB
1-Butanethiol; n-Butyl mercaptan
Heat Capacity 300 K, C_p = 171.39 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 155.76 + 2.780\times10^{-2}T + 8.100\times10^{-5}T^2$.
Molecular Weight 90.1830
Wiswesser Line Notation SH4
Evaluation B

$C_4H_{10}Zn$ (liq) 87GIB/GRI
Diethyl zinc
Heat Capacity 298.15 K, C_p = 188.9 J·mol^{-1}·K^{-1}
Temperature range 18 to 273 K.
Entropy 298.15 K, S = 276.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 239.80 K, ΔH = 18050 J·mol^{-1}
ΔS = 75.30 J·mol^{-1}·K^{-1}
Molecular Weight 123.5030
Wiswesser Line Notation 2-ZN-2
Evaluation A

$C_4H_{10}Zn$ (liq) 88RAB/NIS
Diethyl zinc
Heat Capacity 298.15 K, C_p = 194.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 290.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 148.4 K, ΔH = 275.4 J·mol^{-1}
ΔS = 2.12 J·mol^{-1}·K^{-1}
c,I/liq 236.98 K, ΔH = 16634 J·mol^{-1}
ΔS = 70.19 J·mol^{-1}·K^{-1}
Molecular Weight 123.5030
Wiswesser Line Notation 2-ZN-2
Evaluation A

$C_4H_{11}NO$ (liq) 84GEI/KAR
3-Methoxypropylamine
Heat Capacity 298.15 K, C_p = 225.52 J·mol^{-1}·K^{-1}
Temperature Range 55 to 300 K
Entropy 298.15 K, S = 257.6 J·mol^{-1}·K^{-1}
Phase Changes
Molecular Weight 89.1370
Wiswesser Line Notation Z301
Evaluation B

$C_4H_{11}NO_2$ (c) 82MIN/SAB
Diethanolamine
Heat Capacity 298.15 K, C_p = 137 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 1.3 J·K^{-1}·g^{-1}, an estimated value.
Molecular Weight 105.1364
Wiswesser Line Notation Q2M2Q
Evaluation C

$C_4H_{11}N_3O_7$ (c) 85TAR/SAV
Diglycine nitrate
Heat Capacity 298.15 K, C_p = 297 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
Data given graphically.
$C_p = -0.0108 + 0.231\times10^{-2}T - 0.631\times10^{-5}T^2 + 0.830\times10^{-8}T^3$ cal·g^{-1}·K^{-1} (80 to 300 K).
C_p value calculated from equation.
Phase Changes
c,II/c,I 206.5 K, ΔH = 1072 J·mol^{-1}
ΔS = 5.19 J·mol^{-1}·K^{-1}
Molecular Weight 213.1468
Wiswesser Line Notation Z1VQ 2 &WNQ
Evaluation C

$C_4H_{12}Cl_3MnN$ (c) 83DUN/JEW
Tetramethylammonium trichloromanganate(II)
Heat Capacity 299.55 K, C_p = 240.0 J·mol^{-1}·K^{-1}
Temperature range 1.5 to 300 K.
Value is unsmoothed experimental datum.
Phase Changes
c,II/c,I 126.52 K
Monoclinic-hexagonal.
Molecular Weight 235.4425
Wiswesser Line Notation 1K1&1&1 .MN G3
Evaluation A

$C_4H_{12}Cl_4FeN$ (c) 87RUI/LOP
Tetramethylammonium tetrachloroferrate (III)
Heat Capacity
Temperature range 60 to 350 K.
Data given graphically.
Phase Changes
c,VI/c,V 236.1 K, ΔH = 498.9 J·mol^{-1}
ΔS = 1.98 J·mol^{-1}·K^{-1}
c,V/c,IV 291.4 K, ΔH = 2524 J·mol^{-1}
ΔS = 10.7 J·mol^{-1}·K^{-1}
c,IV/c,III 307.4 K, ΔH = 734.3 J·mol^{-1}
ΔS = 2.38 J·mol^{-1}·K^{-1}
c,III/c,II 347.0 K, ΔH = 713.1 J·mol^{-1}
ΔS = 2.05 J·mol^{-1}·K^{-1}
c,II/c,I 381.0 K, ΔH = 5319.6 J·mol^{-1}
ΔS = 14.0 J·mol^{-1}·K^{-1}
Molecular Weight 271.8045
Wiswesser Line Notation 1K1&1&1 .FE G4
Evaluation A

$C_4H_{12}Ge$ (liq) 70VAL/KIL
Tetramethylgermane
Heat Capacity 300 K, C_p = 196.9 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 300 K, S = 296.80 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 184.368 K, ΔH = 7447.1 J·mol^{-1}
ΔS = 40.39 J·mol^{-1}·K^{-1}
liq/g 285 K, ΔH = 28125 J·mol^{-1}
ΔS = 98.7 J·mol^{-1}·K^{-1}
P = 1 atm
Molecular Weight 132.7288
Wiswesser Line Notation 1-GE-1&1&1
Evaluation A

$C_4H_{12}O_4Si$ (liq) 08KAH/KOE
Tetramethyl silicate; Methyl silicate
Heat Capacity C_p = 319 J·mol^{-1}·K^{-1}
Temperature range 296 to 388 K.
One value given for the entire temperature range.
C_p given as 0.5011 cal·g^{-1}·K^{-1}.
Phase Changes
liq/g 394 K, ΔH = 30900 J·mol^{-1}
ΔS = 78.4 J·mol^{-1}·K^{-1}
Molecular Weight 152.2219
Wiswesser Line Notation 1O-SI-O1&O1&O1
Evaluation D

$C_4H_{12}Pb$ (liq) 54STA/WAR
Tetramethyl lead
Phase Changes
c/liq 242.92 K, ΔH = 10799 J·mol^{-1}
ΔS = 44.43 J·mol^{-1}·K^{-1}
Molecular Weight 267.3388
Wiswesser Line Notation 1-PB-1&1&1
Evaluation B

$C_4H_{12}Sn$ (liq) 54STA/WAR
Tetramethyl tin; Tetramethyl stannane
Phase Changes
c/liq 218.18 K, ΔH = 9439 J·mol^{-1}
ΔS = 43.26 J·mol^{-1}·K^{-1}
Molecular Weight 178.8488
Wiswesser Line Notation 1-SN-1&1&1
Evaluation B

$C_4H_{12}Sn$ (liq) 89SHE/RAB
Tetramethyl tin; Tetramethyl stannane
Heat Capacity 298.15 K, C_p = 197.9 J·mol^{-1}·K^{-1}
Temperature range 5 to 313 K.
Entropy 298.15 K, S = 310.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 218.05 K, ΔH = 9234 J·mol^{-1}
ΔS = 42.35 J·mol^{-1}·K^{-1}
Molecular Weight 178.8488
Wiswesser Line Notation 1-SN-1&1&1
Evaluation A

$C_4H_{13}N_3$ (liq) 88BOB/KAM
Diethylenetriamine
Heat Capacity 313 K, C_p = 254 J·mol^{-1}·K^{-1}
Temperature range 313 to 493 K
Molecular Weight 103.1668
Wiswesser Line Notation Z2M2Z
Evaluation D

$C_4H_{16}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(ethylammonium) manganese II
Phase Changes
c,III/c,II 222 K, $\Delta H = 43.6$ J·mol^{-1}
$\Delta S = 0.20$ J·mol^{-1}·K^{-1}
c,II/c,I 424 K, $\Delta H = 4.1$ J·mol^{-1}
$\Delta S = 0.009$ J·mol^{-1}·K^{-1}
Molecular Weight 288.9338
Wiswesser Line Notation 2ZH2 .MN G4
Evaluation A

C_5F_{12} (liq) 83CAM/DIA
n-Perfluoropentane
Heat Capacity 293 K, $C_p = 188.3$ J·mol^{-1}·K^{-1}
Interpolated data.
Molecular Weight 288.0358
Wiswesser Line Notation FXFFXFFXFFXFFXFFF
Evaluation C

$C_5F_{13}N$ (liq) 84GOL/KOL
Perfluoromethyldiethylamine
Phase Changes
c/liq 150.1 K, $\Delta H = 4600$ J·mol^{-1}
$\Delta S = 30.6$ J·mol^{-1}·K^{-1}
Molecular Weight 321.0409
Wiswesser Line Notation FXFFXFFNXFFF&XFFXFFF
Evaluation A

$C_5H_3F_7O_2$ (liq) 84GOL/KOL
Methyl perfluorobutanoate
Phase Changes
c/liq 191.4 K, $\Delta H = 11770$ J·mol^{-1}
$\Delta S = 61.5$ J·mol^{-1}·K^{-1}
Molecular Weight 228.0663
Wiswesser Line Notation XFFFXFFXFFVO1
Evaluation A

$C_5H_5F_3O_2$ (liq) 84GOL/KOL
Trifluoromethyl (2-hydroxy-1-propenyl) ketone
Phase Changes
c/liq 232.4 K, $\Delta H = 8450$ J·mol^{-1}
$\Delta S = 36.4$ J·mol^{-1}·K^{-1}
Molecular Weight 154.0885
Wiswesser Line Notation QY1&U1VXFFF
Evaluation A

C_5H_6 (liq) 77LEB/LIT4
Cyclopentadiene
Heat Capacity 298.15 K, $C_p = 115.3$ J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, $S = 182.7$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.60 K, $\Delta H = 8010$ J·mol^{-1}
$\Delta S = 45.4$ J·mol^{-1}·K^{-1}
Molecular Weight 66.1024
Wiswesser Line Notation L5 AHJ
Evaluation A

$C_5H_6N_2O_2$ (c) 1889EYK
Thymine
Phase Changes
c/liq 321.3 K, $\Delta H = 17510$ J·mol^{-1}
Molecular Weight 126.1146
Wiswesser Line Notation T6MVMVJ E1
Evaluation C

C_5H_7N (liq) 86STE/CHI
N-Methylpyrrole
Heat Capacity 298.15 K, $C_p = 150.06$ J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, $S = 200.48$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.912 K
Molecular Weight 81.1170
Wiswesser Line Notation T5NJ A1
Evaluation A

C_5H_7N (liq) 87MES/TOD
N-Methylpyrrole
Heat Capacity 298.15 K, $C_p = 150.06$ J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, $S = 200.48$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.912 K, $\Delta H = 7824.8$ J·mol^{-1}
$\Delta S = 36.07$ J·mol^{-1}·K^{-1}
Molecular Weight 81.1170
Wiswesser Line Notation T5NJ A1
Evaluation A

C_5H_7N (liq) 88MES/TOD
N-Methylpyrrole
Heat Capacity 298.150 K, $C_p = 150.058$ J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, $S = 200.519$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 216.912 K, $\Delta H = 7824.77$ J·mol^{-1}
Molecular Weight 81.1170
Wiswesser Line Notation T5NJ A1
Evaluation A

$C_5H_7NO_2$ (liq) 87KHO/BUG
Ethyl cyanoacetate
Heat Capacity 298.15 K, $C_p = 220.22$ J·mol^{-1}·K^{-1}
Temperature range 90 to 300 K.
Entropy 298.15 K, $S = 177.45$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 162.5 K
Glass transition.
Transition temperature estimated from graph.
c,I/liq 246.8 K, $\Delta H = 11780$ J·mol^{-1}
$\Delta S = 47.73$ J·mol^{-1}·K^{-1}
Molecular Weight 113.1158
Wiswesser Line Notation NC1VO2
Evaluation A

C_5H_8 (liq) 75LEB/LEB
Methylenecyclobutane
Heat Capacity 298.15 K, $C_p = 133.6$ J·mol^{-1}·K^{-1}
Temperature range 6 to 320 K.
Entropy 298.15 K, $S = 210.6$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 138.621 K, $\Delta H = 5756$ J·mol^{-1}
$\Delta S = 41.6$ J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A

C_5H_8 (liq) 78LEB/TSV
Methylenecyclobutane
Heat Capacity 298.15 K, C_p = 133.6 J·mol^{-1}·K^{-1}
Temperature range 12 to 315 K.
Entropy 298.15 K, S = 210.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 138.62 K, ΔH = 5755 J·mol^{-1}
ΔS = 41.6 J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A

C_5H_8 (liq) 78LEB/TSV2
Methylenecyclobutane
Heat Capacity 298.15 K, C_p = 133.6 J·mol^{-1}·K^{-1}
Temperature range 12 to 315 K.
Entropy 298.15 K, S = 210.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 138.62 K, ΔH = 5755 J·mol^{-1}
ΔS = 41.6 J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation L4YTJ AU1
Evaluation A

$(C_5H_8)_n$ (liq) 76LEB/RAB
Polypentenamer
Heat Capacity
Temperature range 14 to 322 K.
Phase Changes
c/liq 293 K, ΔH = 8075 J·mol^{-1}
ΔS = 27.56 J·mol^{-1}·K^{-1}
100% crystallinity.
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4*/
Evaluation A
T(glass) = 173 K.

$(C_5H_8)_n$ (liq) 76LEB/RAB2
Polypentenamer
Heat Capacity 298.15 K, C_p = 132.5 J·mol^{-1}·K^{-1}
Temperature range 14 to 322 K.
Entropy 298.15 K, S = 149.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 293 K, ΔH = 8080 J·mol^{-1}
ΔS = 27.58 J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4*/
Evaluation A
T(glass) = 173.5 K.

$(C_5H_8)_n$ (gls) 77LEB/LIT3
cis-Polypentenamer
Heat Capacity 298.15 K, C_p = 128.5 J·mol^{-1}·K^{-1}
Temperature range 7 to 325 K.
Entropy 298.15 K, S = 140.4 J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4* -C/
Evaluation A
T(glass) = 158 K, transition from glass to highly elastic phase.

$(C_5H_8)_n$ (gls) 77LEB/RAB3
cis-Polypentenamer
Heat Capacity 300 K, C_p = 130 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Glassy state.
Data given graphically.
Value estimated from graph.
Entropy 300 K, S = 152 J·mol^{-1}·K^{-1}
Highly elastic state.
Phase Changes
c/liq 232 K, ΔH = 5200 J·mol^{-1}
ΔS = 22.4 J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4* -C/
Evaluation B
T(glass) = 156 K.

$(C_5H_8)_n$ (gls) 77LEB/RAB3
trans-Polypentenamer
Heat Capacity 300 K, C_p = 136 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Glassy state.
Data given graphically.
Value estimated from graph.
Entropy 300 K, S = 150 J·mol^{-1}·K^{-1}
Highly elastic state.
Phase Changes
c/liq 310 K, ΔH = 8900 J·mol^{-1}
ΔS = 28.7 J·mol^{-1}·K^{-1}
Molecular Weight 68.1182
Wiswesser Line Notation /*YU4* -T/
Evaluation B
T(glass) = 175 K.

$C_5H_8O_2$ (liq) 71LEB/RAB
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 300 K, C_p = 192.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S = 266.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.59 K, ΔH = 14435 J·mol^{-1}
ΔS = 64.0 J·mol^{-1}·K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 84VAS/PET
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 300 K, C_p = 192.42 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S = 266.2 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 225.59 K
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 85KAR/ABD
Methyl 2-methylpropenoate; Methyl methacrylate
Heat Capacity 298.15 K, C_p = 215.3 J·mol^{-1}·K^{-1}
Temperature range 225 to 350 K.
Equation only.
C_p (J·kg^{-1}·K^{-1}) = 114.1 + 6.8299 T.
C_p data calculated from equation.
Phase Changes
c/liq 225.6 K
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation B

$C_5H_8O_2$ (liq) 85KAR/ABD2
Methyl 2-methylpropenoate; Methyl methacrylate
Phase Changes
c/liq 225.5 K, ΔH = 13451 J·mol^{-1}
ΔS = 59.65 J·mol^{-1}·K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation 1UY1&VO1
Evaluation A

$C_5H_8O_2$ (liq) 69MEL/MER
Acetylacetone, enol form
Heat Capacity 298.15 K, C_p = 208.2 J·mol^{-1}·K^{-1}
Temperature range 80 to 300 K.
C_{sat}(liq) = 0.8978 + 3.964×10^{-3}T J·K^{-1}·g^{-1} (260 to 300 K);
C_{sat}(298.15 K) given as 2.080 J·K^{-1}·g^{-1}.
Entropy 298.15 K, S = 261.4 J·mol^{-1}·K^{-1}
Extrapolated below 90 K.
S(298.15 K) given as 2.611 J·K^{-1}·g^{-1}.
Phase Changes
c/liq 254.8 K, ΔH = 14497 J·mol^{-1}
ΔS = 56.90 J·mol^{-1}·K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation QY1&U1V1
Evaluation A(C_p), B(S)
C_p(solid) = 0.4257 + 3.674×10^{-3} T J·K^{-1}·g^{-1} (90 to 200 K).

$C_5H_8O_2$ (liq) 83LEB/YEV
δ-Valerolactone
Heat Capacity 298.15 K, C_p = 171.6 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S = 219.0 J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 118.1 K, ΔH = 457 J·mol^{-1}
ΔS = 3.88 J·mol^{-1}·K^{-1}
c,III/c,II 122–155 K, ΔH = 310 J·mol^{-1}
ΔS = 2.2 J·mol^{-1}·K^{-1}
c,II/c,I 180–225 K, ΔH = 205 J·mol^{-1}
ΔS = 0.90 J·mol^{-1}·K^{-1}
c,I/liq 262.82 K, ΔH = 10530 J·mol^{-1}
ΔS = 39.46 J·mol^{-1}·K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation T6OVTJ
Evaluation A

$(C_5H_8O_2)_n$ (c) 67PAV/RAB
Poly(methyl methacrylate)
Heat Capacity 298 K, C_p = 125.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 463 K.
C_p = 0.265 + 1.39×10^{-3}T cal·g·°C (20 to 90 °C).
Value calculated from equation.
Molecular Weight 100.1170
Wiswesser Line Notation /*1X*1&VO1/
Evaluation B
T(glass) = 378 K.

$(C_5H_8O_2)_n$ (c) 71LEB/RAB
Poly(methyl methacrylate)
Heat Capacity 300 K, C_p = 131.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, S = 145.1 J·mol^{-1}·K^{-1}
Molecular Weight 100.1170
Wiswesser Line Notation /*1X*1&VO1/
Evaluation B

$C_5H_9LiO_2$ (c) 86FRA/NGE
Lithium n-pentanoate
Heat Capacity 298.15 K, C_p = 224.07 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 198.55 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 209.3 K, ΔH = 665 J·mol^{-1}
ΔS = 3.24 J·mol^{-1}·K^{-1}
c,II/c,I 319.06 K, ΔH = 2745 J·mol^{-1}
ΔS = 16.13 J·mol^{-1}·K^{-1}
Molecular Weight 108.0659
Wiswesser Line Notation OV4 .LI
Evaluation A

C_5H_9N (liq) 01KAH
Valeronitrile
Heat Capacity C_p = 180.8 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K.
Heat capacity is an average value over the temperature range.
Molecular Weight 83.1328
Wiswesser Line Notation NC4
Evaluation D

C_5H_9NO (c) 62KOL/PAU
α-Piperidone
Heat Capacity 295.00 K, C_p = 208.3 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Entropy 298.15 K, S = 164.9 J·mol^{-1}
Phase Changes
c/liq 342.305 K, ΔH = 16096 J·mol^{-1}
ΔS = 33.7 J·mol^{-1}·K^{-1}
Molecular Weight 99.1299
Wiswesser Line Notation T6MVTU
Evaluation B

$C_5H_9NO_4$ (c) 75SAK/SEK
Glutamic acid
Heat Capacity 298 K, C_p = 175.08 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.19 J·g^{-1}·K^{-1}.
Molecular Weight 147.1304
Wiswesser Line Notation QVYZ2VQ
Evaluation B
C_p same for D and L forms.

$C_5H_9O_2Tl$ (c) 76MEI/SEY
Thallium pentanoate
Phase Changes
c,II/c,I 354.6 K, ΔH = 2259 J·mol^{-1}
ΔS = 6.28 J·mol^{-1}·K^{-1}
c,I/liq 455 K, ΔH = 5439 J·mol^{-1}
ΔS = 12.1 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 487 K, ΔH = 3054 J·mol^{-1}
ΔS = 6.28 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 305.4949
Wiswesser Line Notation OV4 .TL
Evaluation B

$C_5H_9O_2Tl$ (c) 84FER/LOP
Thallium pentanoate
Heat Capacity 320 K, C_p = 216 J·mol^{-1}·K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,II/c,I 353.0 K, ΔH = 2104 J·mol^{-1}
ΔS = 5.99 J·mol^{-1}·K^{-1}
c,I/liq 455.0 K, ΔH = 5704 J·mol^{-1}
ΔS = 12.5 J·mol^{-1}·K^{-1}
Solid to mesophase.
Molecular Weight 305.4949
Wiswesser Line Notation OV4 .TL
Evaluation A
Mesophase to isotropic liquid phase change data also given:
488.0 K; ΔH = 3051 J·mol^{-1};
ΔS = 6.24 J·mol^{-1}·K^{-1}.

C_5H_{10} (liq) 83CHA/HAL
3-Methyl-1-butene
Heat Capacity 298.15 K, C_p = 156.1 J·mol^{-1}·K^{-1}
Temperature range 13 to 298 K.
Entropy 298.15 K, S = 253.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 104.71 K, ΔH = 5359 J·mol^{-1}
ΔS = 51.18 J·mol^{-1}·K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 1Y1&1U1
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 83CHA/HAL
2-Methyl-2-butene
Heat Capacity 298.15 K, C_p = 152.8 J·mol^{-1}·K^{-1}
Temperature range 13 to 301 K.
Entropy 298.15 K, S = 251.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 139.40 K, ΔH = 7579 J·mol^{-1}
ΔS = 54.37 J·mol^{-1}·K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2UY1&1
Evaluation A
A reevaluation of the original measured data from:
47TOD/OLI, 30PAR/HUF.

C_5H_{10} (liq) 83CHA/HAL
2-Methyl-1-butene
Heat Capacity 298.15 K, C_p = 157.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 293 K.
Entropy 298.15 K, S = 254.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 135.60 K, ΔH = 7911 J·mol^{-1}
ΔS = 58.34 J·mol^{-1}·K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 2Y1&U1
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 83CHA/HAL
cis-2-Pentene
Heat Capacity 298.15 K, C_p = 151.8 J·mol-1·K^{-1}
Temperature range 13 to 295 K.
Entropy 298.15 K, S = 258.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 121.78 K, ΔH = 7112 J·mol^{-1}
ΔS = 58.40 J·mol^{-1}·K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 3U2−C
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 83CHA/HAL
trans-2-Pentene
Heat Capacity 298.15 K, C_p = 157.0 J·mol^{-1}·K^{-1}
Temperature range 12 to 302 K.
Entropy 298.15 K, S = 256.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 132.93 K, ΔH = 8352 J·mol^{-1}
ΔS = 62.83 J·mol^{-1}·K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 3U2−T
Evaluation A
A reevaluation of the original measured data from: 47TOD/OLI.

C_5H_{10} (liq) 49SCH/SAG
1-Pentene
Heat Capacity 294 K, C_p = 154.3 J·mol^{-1}·K^{-1}
Temperature range 294 to 378 K.
C_p given as 0.526 Btu(lb)$^{-1}$(°R)$^{-1}$ at 70°F.
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation B

C_5H_{10} (liq) 83CHA/HAL
1-Pentene
Heat Capacity 298.15 K, C_p = 154 J·mol^{-1}·K^{-1}
Temperature range 12 to 353 K.
Entropy 298.15 K, S = 262.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 107.90 K, ΔH = 5807 J·mol^{-1}
ΔS = 53.82 J·mol^{-1}·K^{-1}
Molecular Weight 70.1340
Wiswesser Line Notation 4U1
Evaluation A
A reevaluation of the original measured data from:
47TOD/OLI, 49SCH/SAG.

$C_5H_{10}O$ (liq) 88BAG/GUR
2-Methyl-3-buten-2-ol
Heat Capacity 298.05 K, C_p = 241.2 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 86.1334
Wiswesser Line Notation 1XQ1U1
Evaluation B

$C_5H_{10}O$ (liq) 70HAR/HEA
3-Methyl-2-butanone; Isopropyl methyl ketone
Heat Capacity 298.15 K, C_p = 180.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 1Y1&V1
Evaluation B

$C_5H_{10}O$ (liq) 70HAR/HEA
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p = 200.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 84GRO/BEN
3-Pentanone; Diethyl ketone
Heat Capacity 298.15 K, C_p = 190.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 88BAG/GUR
3-Pentanone; Diethylketone
Heat Capacity 298.15 K, C_p = 196.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 86.1334
Wiswesser Line Notation 2V2
Evaluation B

$C_5H_{10}O$ (liq) 70HAR/HEA
2-Pentanone; *n*-Propyl methyl ketone
Heat Capacity 298.15 K, C_p = 184.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 86.1334
Wiswesser Line Notation 3V1
Evaluation B

$C_5H_{10}O$ (liq) 82DYA/VAS
Valeraldehyde; *n*-Pentanal; Valeral
Entropy 298.15 K, S = 273.6 J·mol^{-1}·K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation B

$C_5H_{10}O$ (liq) 83KOR/DYA
Valeraldehyde; *n*-Pentanal; Valeral
Heat Capacity 298.15 K, C_p = 174.39 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S = 273.59 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 191.59 K
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation B

$C_5H_{10}O$ (liq) 84VAS/PET
Valeral; *n*-Pentanal; Valeraldehyde
Heat Capacity 298.15 K, C_p = 174.39 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S = 273.59 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 191.59 K
Molecular Weight 86.1334
Wiswesser Line Notation VH4
Evaluation A

$C_5H_{10}O$ (liq) 83KOR/DYA
2,2-Dimethylpropanal; Pivalaldehyde
tert-Butylaldehyde
Heat Capacity 298.15 K, C_p = 185.58 J·mol^{-1}·K^{-1}
Temperature range 50 to 350 K.
Entropy 298.15 K, S = 262.05 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 274.15 K
Second order transitions observed at 62.5, 69.0, 110.8, 162.5, and 183.3 K.
Molecular Weight 86.1334
Wiswesser Line Notation VHX1&1&1
Evaluation C

$C_5H_{10}O$ (liq) 88WHI/PER
2,2-Dimethylpropanal; Pivalaldehyde;
tert-Butylaldehyde
Heat Capacity 298.43 K, C_p = 192.8 J·mol^{-1}·K^{-1}
Temperature range 29 to 298 K.
Value is unsmoothed experimental datum.
Phase Changes
c,III/c,II 158.5 K, ΔH = 499 J·mol^{-1}
ΔS = 3.34 J·mol^{-1}·K^{-1}
c,II/c,I 183.9 K, ΔH = 4809 J·mol^{-1}
ΔS = 26.22 J·mol^{-1}·K^{-1}
c,I/liq 272.1 K, ΔH = 2520 J·mol^{-1}
ΔS = 9.3 J·mol^{-1}·K^{-1}
Molecular Weight 86.1334
Wiswesser Line Notation VHX1&1&1
Evaluation C_p(B), transitions (A).

$C_5H_{10}O_2$ (liq) 86JIM/ROM
Ethyl propionate; Ethyl propanoate
Heat Capacity 298.15 K, C_p = 200.90 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 2VO2
Evaluation B

$C_5H_{10}O_2$ (liq) 87ZAB/HYN
Ethyl propionate; Ethyl propanoate
Heat Capacity 298.33 K, C_p = 199.58 J·mol^{-1}·K^{-1}
Temperature range 294 to 349 K.
Unsmoothed experimental datum.
Molecular Weight 102.1328
Wiswesser Line Notation 2VO2
Evaluation B

$C_5H_{10}O_2$ (liq) 86JIM/ROM
Propyl ethanoate; *n*-Propyl acetate
Heat Capacity 298.15 K, C_p = 196.07 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 30V1
Evaluation B

$C_5H_{10}O_2$ (liq) 86JIM/ROM
n-Butyl methanoate
Heat Capacity 298.15 K, C_p = 200.25 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 102.1328
Wiswesser Line Notation 4OVH
Evaluation B

$C_5H_{10}O_3$ (liq) 83SAN/CIO
2-Methoxyethanol acetate
Heat Capacity 298.15 *K* C_p = 310 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K
C_p°(kJ kg^{-1}K^{-1}) = 0.024460T - 4.667
Molecular Weight 118.1322
Wiswesser Line Notation 1V0201
Evaluation D

$C_5H_{10}O_5$ (c) 81KAW/KUS
Xylose(D)
Heat Capacity 303 K, C_p = 184 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ
−A&BCE −B&D
Evaluation B

$C_5H_{10}O_5$ (c) 81KAW/KUS
Arabinose(L)
Heat Capacity 303 K, C_p = 184 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ
−A&C −B&BDE
Evaluation B

$C_5H_{10}O_5$ (c) 81KAW/KUS
Arabinose(D)
Heat Capacity 303 K, C_p = 184 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ
−A&DE −B&BC
Evaluation B

$C_5H_{10}O_5$ (c) 81KAW/KUS
Ribose(D)
Heat Capacity 303 K, C_p = 187 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 150.1310
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ
=A&CDE −B&B
Evaluation B

$C_5H_{11}N$ (liq) 86STE/CHI
3-Methylpyrrolidine
Heat Capacity 298.15 K, C_p = 188.28 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 236.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 170.402 K
Molecular Weight 85.1486
Wiswesser Line Notation T5MTJ C1
Evaluation A

$C_5H_{11}N$ (liq) 86STE/CHI
Piperidine
Heat Capacity 298.15 K, C_p = 179.86 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S = 209.94 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 262.124 K
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation A

$C_5H_{11}N$ (liq) 87MES/TOD
Piperidine
Heat Capacity 298.15 K, C_p = 179.85 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S = 209.94 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 262.124 K, ΔH = 14847.9 J·mol^{-1}
ΔS = 56.64 J·mol^{-1}·K^{-1}
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation A

$C_5H_{11}N$ (liq) 88MES/TOD
Piperidine
Heat Capacity 298.150 K, C_p = 179.857 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S = 209.972 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 262.124 K, ΔH = 14853.69 J·mol^{-1}
ΔS = 56.67 J·mol^{-1}·K^{-1}
Molecular Weight 85.1486
Wiswesser Line Notation T6MTJ
Evaluation A

$C_5H_{11}NO$ (liq) 89ABB/JIM
2,2-Dimethylpropanamide
Heat Capacity 298.150 K, C_p = 159.8 J·mol^{-1}·K^{-1}
One temperature; C_p given as 1.58 J·g^{-1}·K^{-1}.
Phase Changes
c/g 298.15 K, ΔH = 86600 J·mol^{-1}
ΔS = 290.5 J·mol^{-1}·K^{-1}
Molecular Weight 101.1480
Wiswesser Line Notation ZVX1&1&1
Evaluation A

$C_5H_{11}NO_2$ (c) 84GRU/BOU
Norvaline (L); α-Aminovaleric acid (L)
Phase Changes
c,II/c,I 273 K, ΔH = 40 J·mol^{-1}
ΔS = 0.16 J·mol^{-1}·K^{-1}
Molecular Weight 117.1474
Wiswesser Line Notation QVYZ3 -L
Evaluation B

$C_5H_{11}NO_2$ (c) 83SKO/SAB
5-Aminopentanoic acid
Heat Capacity 298 K, C_p = 163.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 117.1474
Wiswesser Line Notation Z4VQ
Evaluation B

$C_5H_{11}NO_2S$ (c) 84GRU/BOU
Methionine (L)
Phase Changes
c,III/c,II 307 K, ΔH = 1980 J·mol^{-1}
ΔS = 6.45 J·mol^{-1}·K^{-1}
c,II/c,I 393 K, ΔH = 150 J·mol^{-1}
ΔS = 0.38 J·mol^{-1}·K^{-1}
Molecular Weight 149.2074
Wiswesser Line Notation QVYZ2S1 -L
Evaluation B

$C_5H_{11}NO_2S$ (c) 84GRU/BOU
Methionine (DL)
Phase Changes
c,III/c,II 326 K, ΔH = 820 J·mol^{-1}
ΔS = 2.51 J·mol^{-1}·K^{-1}
c,II/c,I 380 K
Molecular Weight 149.2074
Wiswesser Line Notation QVYZ2S1
Evaluation B

$C_5H_{12}N_2O$ (c) 87DEL/FER
1,3-Diethylurea
Phase Changes
c,II/c,I 339.4 K, ΔH = 1870 J·mol^{-1}
ΔS = 55.1 J·mol^{-1}·K^{-1}
c/liq 383.4 K, ΔH = 12460 J·mol^{-1}
ΔS = 32.5 J·mol^{-1}·K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation 2MVM2
Evaluation A

$C_5H_{12}N_2O$ (c) 87DEL/FER
Butylurea; Monobutylurea
Phase Changes
c,III/c,II 313.1 K, ΔH = 7020 J·mol^{-1}
c,II/c,I 344.9 K, ΔH = 880 J·mol^{-1}
c/liq 369.3 K, ΔH = 14550 J·mol^{-1}
ΔS = 39.4 J·mol^{-1}·K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVM4
Evaluation A

$C_5H_{12}N_2O$ (c) 87DEL/FER
tert-Butylurea; Mono-*tert*-butylurea
Phase Changes
c/liq 449.8 K, ΔH = 33130 J·mol^{-1}
ΔS = 73.6 J·mol^{-1}·K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVMX
Evaluation A

$C_5H_{12}N_2O$ (c) 86KRA/KOZ
N,N-Diethylurea; 1,1-Diethylurea
Heat Capacity 300 K, C_p = 185.2 J·mol^{-1}·K^{-1}
Temperature range 140–310 K.
Phase Changes
c,II/c,I 195–225 K, ΔH = 2000 J·mol^{-1}
ΔS = 9.61 J·mol^{-1}·K^{-1}
Reversible transition.
c,I/liq 384.43 K, ΔH = 16100 J·mol^{-1}
ΔS = 41.9 J·mol^{-1}·K^{-1}
c/g 326 K, ΔH = 96800 J·mol^{-1}
ΔS = 296.9 J·mol^{-1}·K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVN2&2
Evaluation B

$C_5H_{12}N_2O$ (c) 87DEL/FER
N,N-Diethylurea; 1,1-Diethylurea
Phase Changes
c/liq 342.3 K, ΔH = 16780 J·mol^{-1}
ΔS = 49.0 J·mol^{-1}·K^{-1}
Molecular Weight 116.1626
Wiswesser Line Notation ZVN2&2
Evaluation A

$C_5H_{12}O$ (liq) 75FEN/HAR
3,3-Dimethyl-2-oxabutane; Methyl *tert*-butyl ether
Heat Capacity 298.15 K, C_p = 187.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 1X1&1&O1
Evaluation B

$C_5H_{12}O$ (liq) 75FEN/HAR
3-Oxahexane; Ethyl *n*-propyl ether
Heat Capacity 298.15 K, C_p = 197.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 3O2
Evaluation B

$C_5H_{12}O$ (liq) 75FEN/HAR
2-Oxahexane; Methyl *n*-butyl ether
Heat Capacity 298.15 K, C_p = 193.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 4O1
Evaluation B

$C_5H_{12}O$ (liq) 82VIL/CAS
Methyl *n*-butyl ether; 2-Oxahexane
Heat Capacity 298.15 K, C_p = 192.48 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation 4O1
Evaluation B

$C_5H_{12}O$ (liq) 76SKO/SUU
1-Pentanol; *n*-Amyl alcohol; *n*-Pentyl alcohol
Heat Capacity 298.15 K, C_p = 208.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation A

$C_5H_{12}O$ (liq) 83DAP/DEL
1-Pentanol; *n*-Amyl alcohol; *n*-Pentyl alcohol
Heat Capacity 298.15 K, C_p = 207.4 J·mol^{-1}·K^{-1}
Data given at 288 and 298 K.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 84ZEG/SOM
1-Pentanol; *n*-Amyl alcohol; *n*-Pentyl alcohol
Heat Capacity 298.15 K, C_p = 208.98 J·mol^{-1}·K^{-1}
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation B

$C_5H_{12}O$ (liq) 86TAN/TOY
1-Pentanol; *n*-Amyl alcohol; *n*-Pentyl alcohol
Heat Capacity 298.15 K, C_p = 208.19 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation Q5
Evaluation A

$C_5H_{12}O$ (liq) 83DAP/DEL
2-Methyl-2-butanol; *tert*-Pentanol;
tert-Pentyl alcohol
Heat Capacity 298.15 K, C_p = 247.3 J·mol^{-1}·K^{-1}
Data given at 288 and 298 K.
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B

$C_5H_{12}O$ (liq) 88PIE/SOM
2-Methyl-2-butanol; *tert*-Pentanol;
tert-Pentyl alcohol
Heat Capacity 298.15 K, C_p = 247.15 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 88.1492
Wiswesser Line Notation QX1&1&2
Evaluation B

$C_5H_{12}O_2$ (liq) 88BAG/GUR
2,2-Dimethoxypropane
Heat Capacity 298.15 K, C_p = 217.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 104.1486
Wiswesser Line Notation 1OXO1
Evaluation B

$C_5H_{12}O_4$ (c) 50HOS/NAG
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Phase Changes
c,II/c,I 457 K, ΔH = 35146 J·mol^{-1}
ΔS = 76.9 J·mol^{-1}·K^{-1}
c,I/liq 529 K, ΔH = 5439 J·mol^{-1}
ΔS = 10.28 J·mol^{-1}·K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation B

$C_5H_{12}O_4$ (c) 89ZHA/YAN
2,2-Bis(hydroxymethyl)-1,3-dihydroxypropane; Pentaerythritol
Heat Capacity 298.98 *K* 188.40 J·mol^{-1}·K^{-1}
Temperature range 277 to 510 K
Phase Changes
c,II/c,I 461.60 K ΔH = 41380 *J* mol^{-1}
ΔS = 89.64 J·mol^{-1}·K^{-1}
Molecular Weight 136.1474
Wiswesser Line Notation Q1X1Q1Q1Q
Evaluation A

$C_5H_{12}Si$ (liq) 75RAB/LEB
Vinyltrimethylsilane
Heat Capacity 300 K, C_p = 198.3 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 300 K, S = 313.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 141.65 K, ΔH = 7657 J·mol^{-1}
ΔS = 54.06 J·mol^{-1}·K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation 1U1-SI-1&1&1
Evaluation A

$C_5H_{12}Si$ (liq) 81LEB/LEB
Vinyltrimethylsilane
Heat Capacity 298.15 K, C_p = 198.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 312.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 141.57 K, ΔH = 7660 J·mol^{-1}
ΔS = 54.0 J·mol^{-1}·K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation 1U1-SI-1&1&1
Evaluation A

$C_5H_{12}Si$ (c) 75GUS/KAR
1,1-Dimethyl-1-silacyclobutane
Heat Capacity 298.15 K, C_p = 197.53 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Data given graphically.
Entropy 298.15 K, S = 279.49 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 155.52 K, ΔH = 6761 J·mol^{-1}
ΔS = 43.51 J·mol^{-1}·K^{-1}
liq/g 355.91 K, ΔH = 32141 J·mol^{-1}
ΔS = 90.29 J·mol^{-1}·K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation T4-SI-TJ A1 A1
Evaluation B

$(C_5H_{12}Si)n$ (gls) 75RAB/LEB
Polyvinyltrimethylsilane
Heat Capacity 300 K, C_p = 179.9 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 300 K, S = 217.6 J·mol^{-1}·K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation /*1Y*-SI-1&1&1/
Evaluation A

$(C_5H_{12}Si)_n$ (c) 81LEB/LEB
Polyvinyltrimethylsilane
Heat Capacity 298.15 K, C_p = 166.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 189.6 J·mol^{-1}·K^{-1}
Molecular Weight 100.2353
Wiswesser Line Notation /*1Y*-SI-1&1&1/

$C_5H_{13}N$ (liq) 01KAH
1-Aminopentane; *n*-Amylamine; *n*-Pentylamine
Heat Capacity C_p = 223.8 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K.
Heat capacity is an average value over the temperature range.
Molecular Weight 87.1644
Wiswesser Line Notation Z5
Evaluation D

$C_5H_{13}NO$ (liq) 81LEB/RYA
Methylethylethanolamine
Heat Capacity C_p = 256.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 343 K.
Heat capacity is an average value over the temperature range.
Molecular Weight 103.1638
Wiswesser Line Notation Q2N2&1
Evaluation B

$C_5H_{14}N_2$ (liq) 84LEB/GUT
N,N-Dimethyl-1,3-propanediamine
Heat Capacity 298 K, C_p = 248.71 J·mol^{-1}·K^{-1}
Temperature range 295 to 360 K.
Phase Changes
liq/g 406 K
P = 9.972×10^4 kPa.
Molecular Weight 102.1790
Wiswesser Line Notation Z3N1&1
Evaluation B
ΔH vaporization = 44100 J·mol^{-1}, temperature range = 290 to 317 K.

$C_5H_{14}N_2O$ (liq) 88KOZ/KRA
Tetramethylurea
Heat Capacity 320 K, C_p = 241.2 J·mol^{-1}·K^{-1}
Temperature range 160 to 425 K. Equation only.
C_p(c) = 60.22 + 0.520 T J·mol^{-1}·K^{-1} (160 to 240K);
C_p(liq) = 153.30 + 0.2748 J·mol^{-1}·K^{-1} (320 to 425K).
Phase Changes
c/liq 272.2 K, ΔH = 13400 J·mol^{-1}
ΔS = 49.2 J·mol^{-1}·K^{-1}
Molecular Weight 118.1784
Wiswesser Line Notation 1M1&VM1&1
Evaluation A

$C_5H_{15}N_3$ (liq) 81LEB/RYA
Dimethylaminopropylenediamine
Heat Capacity 295.96 K, C_p = 249.0 J·mol^{-1}·K^{-1}
Temperature range 296 to 359 K.
Molecular Weight 117.1936
Wiswesser Line Notation Z1Y1ZN1&1
Evaluation B

$C_5H_{16}Cl_4Mn$ (c) 88CHH/ABE
Pentyldiamine manganese tetrachloride
Heat Capacity 298.15 K, C_p = 424.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S = 407.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 299.6 K, ΔH = 2240 J·mol^{-1}
ΔS = 8.3 J·mol^{-1}·K^{-1}
Molecular Weight 272.9314
Wiswesser Line Notation Z5Z &GH 2 .MN G2

$C_6Br_2Cl_3F_9$ (liq) 88SVO/VES
1,6-Dibromo-2,3,5-trichlorononafluorohexane
Heat Capacity 298.16 K, C_p = 418.6 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 318.15 K.
C_p (J·mol^{-1}·K^{-1}) = 335.6 + 0.278 (T/K)(298–318 K).
Molecular Weight 509.2186
Wiswesser Line Notation FXFEXGFXGFXFFXGFXFFE
Evaluation A

$C_6D_{17}BeF_4N_3O_6$ (c) 79LOI/OSB
Triglycine fluoroberyllate, deuterated
Heat Capacity 300 K, C_p = 447.4 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K.
C_p = 0.326 cal·g^{-1}·K^{-1}, 92% deuterated.
Phase Changes
c,II/c,I ΔH = 1153 J·mol^{-1}
No temperature given.
Molecular Weight 327.9862
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4 &1/H-2 2 &2/H-2 2 &4/H-2 1 &9/H-2 2
Evaluation B

$C_6D_{17}BeF_4N_3O_6$ (c) 81LOI/KOS
Triglycine fluoroberyllate, deuterated
Heat Capacity 308 K, C_p = 448 J·mol^{-1}·K^{-1}
One temperature.
C_p(35 °C) = 0.33 cal·g^{-1}· °C^{-1}.
Molecular Weight 324.2166
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4 &1/H-2 2 &2/H-2 2 &4/H-2 1 &9/H-2 2
Evaluation B
70% deuterated.

$C_6D_{17}BeF_4N_3O_6$ (c) 81LOI/KOS2
Triglycine fluoroberyllate, deuterated
Heat Capacity 298 K, C_p = 430 J·mol^{-1}·K^{-1}
Temperature range 294 to 375 K.
C_p given at "room temperature" as 0.317 cal·K^{-1}·g^{-1}.
Data given graphically.
Phase Changes
c,II/c,I 345 K, ΔH = 813 J·mol^{-1}
ΔS = 2.36 J·mol^{-1}·K^{-1}
Ferroelectric transition.
Molecular Weight 324.2166
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4 &1/H-2 2 &2/H-2 2 &4/H-2 1 &9/H-2 2
Evaluation C
Sample is 70% deuterated.

$C_6D_{17}N_3O_{10}S$ (c) 75CAM/GON
Triglycine sulfate, deuterated
Heat Capacity 300 K, C_p = 390 J·mol^{-1}·K^{-1}
Temperature range 100 to 400 K.
Data given graphically; C_p estimated from graph.
Phase Changes
c,II/c,I 331.75 K, ΔH = 571 J·mol^{-1}
ΔS = 1.72 J·mol^{-1}·K^{-1}
Molecular Weight 338.7013
Wiswesser Line Notation Z1VQ 3 &WSQQ &1/H-2 2 &1/H-2 2 &4/H-2 1 &11/H-2 1 &12/H-2 1
Evaluation D(C_p); B(Phase changes)
Degree of deuteration not indicated, assumed 90%.

$C_6D_{17}N_3O_{10}S$ (c) 79LOI/OSB
Triglycine sulfate, deuterated
Heat Capacity 300 K, C_p = 438 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K.
C_p = 0.309 cal·g^{-1}·K^{-1}.
90% deuterated.
Molecular Weight 338.7013
Wiswesser Line Notation Z1VQ 3 &WSQQ &1/H-2 2 &1/H-2 2 &4/H-2 1 &11/H-2 1 &12/H-2 1
Evaluation B

$C_6D_{17}N_3O_{10}S$ (c) 81LOI/KOS
Triglycine sulfate, deuterated
Heat Capacity 308 K, C_p = 468 J·mol^{-1}·K^{-1}
One temperature.
C_p(35 °C) = 0.33 cal·g^{-1}· °C^{-1}.
Molecular Weight 338.7013
Wiswesser Line Notation Z1VQ 3 &WSQQ &1/H-2 2 &1/H-2 2 &4/H-2 1 &11/H-2 1 &12/H-2 1
Evaluation B
90% deuterated.

C_6F_6 (liq) 82GOR/SIM
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.76 K, C_p = 221.3 J·mol^{-1}·K^{-1}
Temperature range 284 to 350 K.
Value is unsmoothed experimental datum.
C_p (298.76 K) given as 1.1892 J·K^{-1}·g^{-1}.
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CD DF EF FF
Evaluation B
C_p(liq) (kJ·kg^{-1}·K^{-1}) = 1.19132 − 1.0716×10^{-3} T + 3.59×10^{-6} T^2 J·K^{-1}·g^{-1} (325 to 728 K).

C_6F_6 (liq) 82GOR/SIM2
Hexafluorobenzene; Perfluorobenzene
Heat Capacity 298.15 K, C_p = 221.6 J·mol^{-1}·K^{-1}
Temperature range 280 to 680 K.
Data calculated from the equation:
C_p(liq) (kJ·kg^{-1}·K^{-1}) = 1.19132 − 1.0716×10^{-3}T + 3.59×10$^{-6}T^2$.
Molecular Weight 186.0564
Wiswesser Line Notation FR BF CF DF EF FF
Evaluation A

C_6F_{14} (liq) 83CAM/DIA
n-Perfluorohexane
Heat Capacity 273 K, C_p = 240.2 J·mol^{-1}·K^{-1}
Data from 82CAM/REY.
Molecular Weight 338.0436
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFF
Evaluation C
C_p given as 248.1 J·mol^{-1}·K^{-1} at 273 K from Cochran, M.A. et al, J. Chem. Soc. Faraday Trans. **70**, 1274 (1974).

$C_6F_{15}N$ (liq) 84GOL/KOL
Perfluorotriethylamine
Phase Changes
c/liq 156.1 K, ΔH = 4650 J·mol^{-1}
ΔS = 29.8 J·mol^{-1}·K^{-1}
Molecular Weight 371.0487
Wiswesser Line Notation FXFFXFF 3N
Evaluation A

$C_6H_2Cl_4$ (c) 82MAR
1,2,4,5-Tetrachlorobenzene
Phase Changes
c,II/c,I 187.5 K, ΔH = 34 J·mol^{-1}
ΔS = 0.18 J·mol^{-1}·K^{-1}
Molecular Weight 215.8938
Wiswesser Line Notation GR BG DG EG
Evaluation C

$C_6H_3Br_3O$ (c) 87ALL/FIN
2,4,6-Tribromophenol
Heat Capacity 298.15 K, C_p = 172.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.52 J.K^{-1}.g^{-1}.
Molecular Weight 330.8011
Wiswesser Line Notation QR BE DE FE
Evaluation B

$C_6H_3Cl_3$ (liq) 86WIL/LAI
1,2,4-Trichlorobenzene
Heat Capacity 298.15 K, C_p = 194.90 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 181.4487
Wiswesser Line Notation GR BG DG
Evaluation B

$C_6H_3Cl_4N$ (c) 87TAN/YEJ
2-Chloro-1-(trichloromethyl)pyridine
Heat Capacity 297.13 K, C_p = 192.09 J·mol^{-1}·K^{-1}
Temperature range 78 to 322 K.
Value is unsmoothed experimental datum.
C_p(c,70to330K) = 146.438 + 57.0749X− 1.31699×^{2}
+ 16.2918×^{3} − 11.3899×^{4}− 26.7611X^5 + 5.59976X^6
+ 21.3037X^7 (J·mol^{-1}·K^{-1}).
Phase Changes
c/liq 337.242 K, ΔH = 20298.8 J·mol^{-1}
ΔS = 60.190 J·mol^{-1}·K^{-1}
Molecular Weight 230.9084
Wiswesser Line Notation T6NJ BXGGG FG
Evaluation B

$C_6H_3N_3O_7$ (c) 79FAR/SHA
Picric acid; 2,4,6-Trinitrophenol
Phase Changes
c/liq 394.1 K, ΔH = 17100 J·mol^{-1}
ΔS = 43.4 J·mol^{-1}·K^{-1}
Molecular Weight 229.1056
Wiswesser Line Notation WNR BQ CNW ENW
Evaluation B

$C_6H_3N_3O_8$ (c) 79FAR/SHA
Styphnic acid; 2,4,6-Trinitroresorcinol
Phase Changes
c/liq 454.9 K, ΔH = 33500 J·mol^{-1}
ΔS = 73.6 J·mol^{-1}·K^{-1}
Molecular Weight 245.1050
Wiswesser Line Notation WNR BQ CNW DQ ENW
Evaluation B

C_6H_4BrCl (liq) 18NAR
2-Chlorobromobenzene
Heat Capacity 298.15 K, C_p = 176.9 J·mol^{-1}·K^{-1}
Temperature range 198 to 374 K.
C_p = 0.21497 + 0.0002348t cal·g^{-1}·K^{-1}.
C_p value calculated from equation.
Phase Changes
c/liq 260.55 K, ΔH = 12368 J·mol^{-1}
ΔS = 47.5 J·mol^{-1}·K^{-1}
Molecular Weight 191.4546
Wiswesser Line Notation GR BE
Evaluation D

C_6H_4BrCl (liq) 18NAR
3-Chlorobromobenzene
Heat Capacity 298.15 K, C_p = 181.9 J·mol^{-1}·K^{-1}
Temperature range 197 to 375 K.
C_p = 0.221224 + 0.0002348 t cal·g^{-1}·K^{-1}.
C_p value calculated from equation.
Phase Changes
c/liq 251.95 K, ΔH = 12288 J·mol^{-1}
ΔS = 48.8 J·mol^{-1}·K^{-1}
Molecular Weight 191.4546
Wiswesser Line Notation GR CE
Evaluation D

C_6H_4BrCl (c) 18NAR
4-Chlorobromobenzene
Heat Capacity
Temperature range 194 to 336 K.
Phase Changes
c/liq 337.75 K, ΔH = 18760 J·mol^{-1}
ΔS = 55.5 J·mol^{-1}·K^{-1}
Molecular Weight 191.4546
Wiswesser Line Notation GR DE
Evaluation D

C_6H_4BrI (liq) 18NAR
2-Bromoiodobenzene
Heat Capacity 298.15 K, C_p = 179.9 J·mol^{-1}·K^{-1}
Temperature range 195 to 373 K.
C_p = 0.15285 + 0.0001332t.
C_p value calculated from equation.
Phase Changes
c/liq 275.25 K, ΔH = 14441 J·mol^{-1}
ΔS = 52.5 J·mol^{-1}·K^{-1}
Molecular Weight 282.9061
Wiswesser Line Notation IR BE
Evaluation D

C_6H_4BrI (liq) 18NAR
3-Bromoiodobenzene
Heat Capacity 298.15 K, C_p = 183.1 J·mol^{-1}·K^{-1}
Temperature range 198 to 373 K.
C_p = 0.15134 + 0.0001332t.
C_p value calculated from equation.
Phase Changes
c/liq 263.85 K, ΔH = 12192 J·mol^{-1}
ΔS = 46.2 J·mol^{-1}·K^{-1}
Molecular Weight 282.9061
Wiswesser Line Notation IR CE
Evaluation D

C_6H_4BrI (c) 18NAR
4-Bromoiodobenzene
Heat Capacity
Temperature range 270 to 361 K.
Phase Changes
c/liq 363.25 K, ΔH = 19614 J·mol^{-1}
ΔS = 54.0 J·mol^{-1}·K^{-1}
Molecular Weight 282.9061
Wiswesser Line Notation IR DE
Evaluation D

$C_6H_4Br_2$ (liq) 18NAR
1,2-Dibromobenzene
Heat Capacity 298.15 K, C_p = 196.8 J·mol^{-1}·K^{-1}
Temperature range 200 to 375 K.
C_p = 0.17994 + 0.0002140t.
C_p value calculated from equation.
Phase Changes
c/liq 274.95 K, ΔH = 13587 J·mol^{-1}
ΔS = 49.4 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER BE
Evaluation D

$C_6H_4Br_2$ (liq) 18NAR
1,3-Dibromobenzene
Heat Capacity 298.15 K, C_p = 192.0 J·mol^{-1}·K^{-1}
Temperature range 197 to 375 K.
C_p = 0.17535 + 0.0002140t.
C_p value calculated from equation.
Phase Changes
c/liq 266.25 K, ΔH = 14225 J·mol^{-1}
ΔS = 53.4 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER CE
Evaluation D

$C_6H_4Br_2$ (c) 18NAR
1,4-Dibromobenzene
Heat Capacity
Temperature range 194 to 353 K.
Phase Changes
c/liq 360.05 K, ΔH = 20530 J·mol^{-1}
ΔS = 57.0 J·mol^{-1}·K^{-1}
Molecular Weight 235.9056
Wiswesser Line Notation ER DE
Evaluation D

$C_6H_4Br_3N$ (c) 87ALL/FIN
2,4,6-Tribromoaniline
Heat Capacity 298.15 K, C_p = 181.4 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.55 J.K^{-1}.g^{-1}.
Molecular Weight 329.8163
Wiswesser Line Notation ZR BE DE FE
Evaluation B

$C_6H_4ClNO_2$ (c) 81LEB/RYA
1,2-Chloronitrobenzene
Heat Capacity C_p = 247.8 J·mol^{-1}·K^{-1}
Temperature range 298 to 303 K.
Data given over temperature range.
Molecular Weight 157.5561
Wiswesser Line Notation WNR BG
Evaluation B

$C_6H_4ClNO_2$ (c) 81LEB/RYA
4-Nitrochlorobenzene
Heat Capacity C_p = 182.6 J·mol^{-1}·K^{-1}
Temperature range 298 to 353 K.
Data given over temperature range.
Molecular Weight 157.5561
Wiswesser Line Notation WNR DG
Evaluation B

$C_6H_4ClNO_2$ (c) 81VOR/BOR
4-Nitrochlorobenzene
Phase Changes
c/liq 358 K, ΔH = 18030 J·mol^{-1}
ΔS = 69.9 J·mol^{-1}·K^{-1}
liq/g 518 K, ΔH = 36900 J·mol^{-1}
ΔS = 71.2 J·mol^{-1}·K^{-1}
Molecular Weight 157.5561
Wiswesser Line Notation WNR DG
Evaluation C

$C_6H_4Cl_2$ (liq) 18NAR
1,2-Dichlorobenzene; *o*-Dichlorobenzene
Heat Capacity 298.15 K, C_p = 170.9 J·mol^{-1}·K^{-1}
Temperature range 197 to 375 K.
C_p = 0.27022 + 0.0003024 t cal·g^{-1}·K^{-1}.
C_p value calculated from equation.
Phase Changes
c/liq 255.65 K, ΔH = 12922 J·mol^{-1}
ΔS = 50.5 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR BG
Evaluation D

$C_6H_4Cl_2$ (liq) 18NAR
1,3-Dichlorobenzene; *m*-Dichlorobenzene
Heat Capacity 298.15 K, C_p = 170.9 J·mol^{-1}·K^{-1}
Temperature range 197 to 377 K.
C_p = 0.27022 + 0.0003024 t cal·g^{-1}·K^{-1}.
C_p value calculated from equation.
Phase Changes
c/liq 248.75 K, ΔH = 12590 J·mol^{-1}
ΔS = 50.6 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR CG
Evaluation D

$C_6H_4Cl_2$ (c) 18NAR
1,4-Dichlorobenzene; *p*-Dichlorobenzene
Heat Capacity 298 K, C_p = 147.6 J·mol^{-1}·K^{-1}
Temperature range 194 to 372 K.
Average specific heat over the temperature range 2.6 to 51.6 °C is 0.2400 cal·g^{-1}·K^{-1}.
Phase Changes
c/liq 326.05 K, ΔH = 18144 J·mol^{-1}
ΔS = 55.6 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation D

$C_6H_4Cl_2$ (c) 72BOO/HAU
1,4-Dichlorobenzene; *p*-Dichlorobenzene
Phase Changes
c/liq 326.15 K, ΔH = 18050 J·mol^{-1}
ΔS = 55.3 J·mol^{-1}·K^{-1}
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation C

$C_6H_4Cl_2$ (c,II) 75DWO/FIG
1,4-Dichlorobenzene; *p*-Dichlorobenzene
Heat Capacity
Temperature range 18 to 322 K.
Data given graphically.
Phase Changes

c,III/c,II	271.77 K,	ΔH = 1256 J·mol^{-1}
		ΔS = 4.62 J·mol^{-1}·K^{-1}
c,II/c,I	304.35 K,	ΔH = 214.5 J·mol^{-1}
		ΔS = 0.705 J·mol^{-1}·K^{-1}
c,I/liq	326.14 K,	ΔH = 18187 J·mol^{-1}
		ΔS = 55.76 J·mol^{-1}·K^{-1}

Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation A
See also 76DWO/FIG.

$C_6H_4Cl_2$ (c) 88MAR/MON2
1,4-Dichlorobenzene; *p*-Dichlorobenzene
Heat Capacity 180 K, C_p = 98 J·mol^{-1}·K^{-1}
Temperature range 30 to 180 K.
Data given graphically, and estimated from graph.
Molecular Weight 147.0036
Wiswesser Line Notation GR DG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,3-Dichlorophenol
Phase Changes

c/liq	330.0 K,	ΔH = 21363 J·mol^{-1}
		ΔS = 64.74 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR BG CG
Evaluation A

$C_6H_4Cl_2O$ (c) 81VOR/BOR
2,4-Dichlorophenol
Phase Changes

c/liq	323 K,	ΔH = 28410 J·mol^{-1}
		ΔS = 88.0 J·mol^{-1}·K^{-1}
liq/g	491 K,	ΔH = 36780 J·mol^{-1}
		ΔS = 74.9 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR BG DG
Evaluation C

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,4-Dichlorophenol
Phase Changes

c/liq	318.0 K,	ΔH = 20090 J·mol^{-1}
		ΔS = 63.18 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR BG DG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,5-Dichlorophenol
Phase Changes

c/liq	331.0 K,	ΔH = 22434 J·mol^{-1}
		ΔS = 67.78 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR BG EG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
2,6-Dichlorophenol
Phase Changes

c/liq	340.0 K,	ΔH = 22141 J·mol^{-1}
		ΔS = 65.12 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR BG FG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
3,4-Dichlorophenol
Phase Changes

c/liq	341.0 K,	ΔH = 20927 J·mol^{-1}
		ΔS = 61.37 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR CG DG
Evaluation A

$C_6H_4Cl_2O$ (c) 82POE/FAN
3,5-Dichlorophenol
Phase Changes

c/liq	341.0 K,	ΔH = 20509 J·mol^{-1}
		ΔS = 60.14 J·mol^{-1}·K^{-1}

Molecular Weight 163.0030
Wiswesser Line Notation QR CG EG
Evaluation A

$C_6H_4F_2$ (liq) 62GOO/LAC
1,2-Difluorobenzene
Heat Capacity 298.15 K, C_p = 159.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.0944
Wiswesser Line Notation FR BF
Evaluation B

$C_6H_4F_2$ (liq) 62GOO/LAC
1,3-Difluorobenzene
Heat Capacity 298.15 K, C_p = 157.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.0944
Wiswesser Line Notation FR CF
Evaluation B

$C_6H_4F_2$ (liq) 62GOO/LAC
1,4-Difluorobenzene
Heat Capacity 298.15 K, C_p = 157.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.0944
Wiswesser Line Notation FR DF
Evaluation B

$C_6H_4I_2$ (liq) 18NAR
1,2-Diiodobenzene
Heat Capacity 298.15 K, C_p = 190.0 J·mol^{-1}·K^{-1}
Temperature range 196 to 373 K.
C_p = 0.1357 + 0.0000776t.
C_p value calculated from equation.
Phase Changes

c/liq	296.55 K,	ΔH = 14079 J·mol^{-1}
		ΔS = 47.5 J·mol^{-1}·K^{-1}

Molecular Weight 329.9066
Wiswesser Line Notation IR BI
Evaluation D

$C_6H_4I_2$ (c) 18NAR
1,3-Diiodobenzene
Heat Capacity
Temperature range 196 to 306 K.
Phase Changes
c/liq 307.35 K, $\Delta H = 15943$ J·mol^{-1}
$\Delta S = 51.9$ J·mol^{-1}·K^{-1}
Molecular Weight 329.9066
Wiswesser Line Notation IR CI
Evaluation D

$C_6H_4I_2$ (c) 18NAR
1,4-Diiodobenzene
Heat Capacity
Temperature range 198 to 400 K.
Phase Changes
c/liq 402.15 K, $\Delta H = 22375$ J·mol^{-1}
$\Delta S = 55.6$ J·mol^{-1}·K^{-1}
Molecular Weight 329.9066
Wiswesser Line Notation IR DI
Evaluation D

$C_6H_4N_2O_4$ (c) 72BOO/HAU
1,2-Dinitrobenzene
Phase Changes
c/liq 390.05 K, $\Delta H = 22750$ J·mol^{-1}
$\Delta S = 58.3$ J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR BNW
Evaluation C

$C_6H_4N_2O_4$ (c) 72BOO/HAU
1,3-Dinitrobenzene
Phase Changes
c/liq 363.23 K, $\Delta H = 17350$ J·mol^{-1}
$\Delta S = 47.8$ J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR CNW
Evaluation C

$C_6H_4N_2O_4$ (c) 72BOO/HAU
1,4-Dinitrobenzene
Phase Changes
c/liq 446.65 K, $\Delta H = 28100$ J·mol^{-1}
$\Delta S = 62.9$ J·mol^{-1}·K^{-1}
Molecular Weight 168.1086
Wiswesser Line Notation WNR DNW
Evaluation C

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,3-Dinitrophenol
Phase Changes
c/liq 417.0 K, $\Delta H = 26239$ J·mol^{-1}
$\Delta S = 62.92$ J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR BNW CQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
3,4-Dinitrophenol
Phase Changes
c/liq 407.0 K, $\Delta H = 25376$ J·mol^{-1}
$\Delta S = 62.35$ J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR BNW DQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,6-Dinitrophenol
Phase Changes
c/liq 336.0 K, $\Delta H = 19577$ J·mol^{-1}
$\Delta S = 58.26$ J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR BQ CNW
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,4-Dinitrophenol
Phase Changes
c/liq 388.0 K, $\Delta H = 24174$ J·mol^{-1}
$\Delta S = 62.30$ J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR CNW DQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
3,5-Dinitrophenol
Phase Changes
c/liq 399.1 K
Molecular Weight 184.1080
Wiswesser Line Notation WNR CNW EQ
Evaluation A

$C_6H_4N_2O_5$ (c) 82POE/FAN
2,5-Dinitrophenol
Phase Changes
c/liq 381.0 K, $\Delta H = 23730$ J·mol^{-1}
$\Delta S = 62.28$ J·mol^{-1}·K^{-1}
Molecular Weight 184.1080
Wiswesser Line Notation WNR CQ DNW
Evaluation A

C_6H_5Br (liq) 86RED
Bromobenzene
Heat Capacity 303.15 K, $C_p = 155.9$ J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 157.0095
Wiswesser Line Notation ER
Evaluation B

C_6H_5BrO (c) 1889EYK
4-Bromophenol
Phase Changes
c/liq 336 K, $\Delta H = 16573$ J·mol^{-1}
$\Delta S = 49.3$ J·mol^{-1}·K^{-1}
Molecular Weight 173.0091
Wiswesser Line Notation QR DE
Evaluation C

C_6H_5Cl (liq) 86RED
Chlorobenzene
Heat Capacity 303.15 K, $C_p = 150.6$ J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation B

C_6H_5Cl (liq) 88PER/AIC
Chlorobenzene
Heat Capacity 298.15 K, $C_p = 153.78$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.5585
Wiswesser Line Notation GR
Evaluation A

C_6H_5ClO (liq) 82POE/FAN
2-Chlorophenol
Phase Changes
c/liq 283.0 K, $\Delta H = 12523$ J·mol^{-1}
$\Delta S = 44.25$ J·mol^{-1}·K^{-1}
Molecular Weight 128.5579
Wiswesser Line Notation QR BG
Evaluation A

C_6H_5ClO (c) 82POE/FAN
3-Chlorophenol
Phase Changes
c/liq 305.8 K, $\Delta H = 14905$ J·mol^{-1}
$\Delta S = 48.74$ J·mol^{-1}·K^{-1}
Molecular Weight 128.5579
Wiswesser Line Notation QR CG
Evaluation A

C_6H_5ClO (c) 82POE/FAN
4-Chlorophenol
Phase Changes
c/liq 316.0 K, $\Delta H = 14067$ J·mol^{-1}
$\Delta S = 44.51$ J·mol^{-1}·K^{-1}
Molecular Weight 128.5579
Wiswesser Line Notation QR DG
Evaluation A

$C_6H_5Cl_3Ge$ (c) 69NUR/KOS
Phenyltrichlorogermane
Entropy 298.15 K, $S = 339.9$ J·mol^{-1}·K^{-1}
Deposited in VINITI, No 540–69, 11 March 1969.
Molecular Weight 256.0545
Wiswesser Line Notation G-GE-GGR
Evaluation A

$C_6H_5Cl_3Sn$ (c) 69NUR/KOS
Phenyltrichlorostannane
Entropy 298.15 K, $S = 347.5$ J·mol^{-1}·K^{-1}
Deposited in VINITI, No 540–69, 11 March 1969.
Molecular Weight 302.1545
Wiswesser Line Notation G-SN-GGR
Evaluation A

C_6H_5F (liq) 84ROU/GRO
Fluorobenzene
Heat Capacity 298.15 K, $C_p = 146.29$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1039
Wiswesser Line Notation FR
Evaluation B

$C_6H_5NO_2$ (liq) 86RED
Nitrobenzene
Heat Capacity 303.15 K, $C_p = 177.3$ J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 123.1110
Wiswesser Line Notation WNR
Evaluation B

$C_6H_5NO_3$ (c) 82POE/FAN
2-Nitrophenol
Phase Changes
c/liq 318.0 K, $\Delta H = 17446$ J·mol^{-1}
$\Delta S = 54.86$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR BQ
Evaluation A

$C_6H_5NO_3$ (c) 72BOO/HAU
3-Nitrophenol
Phase Changes
c/liq 369.95 K, $\Delta H = 21300$ J·mol^{-1}
$\Delta S = 57.6$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR CQ
Evaluation C

$C_6H_5NO_3$ (c) 82POE/FAN
3-Nitrophenol
Phase Changes
c/liq 370.0 K, $\Delta H = 19196$ J·mol^{-1}
$\Delta S = 51.88$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR CQ
Evaluation A

$C_6H_5NO_3$ (c) 41CAM/CAM
4-Nitrophenol
Heat Capacity 283 K, $C_p = 144$ J·mol^{-1}·K^{-1}
Temperature range 273 to 293 K.
Value given as
$C_p = 0.248$ cal·g^{-1} over temperature range 0 to 20 °C.
Phase Changes
c/liq 387 K, $\Delta H = 24271$ J·mol^{-1}
$\Delta S = 62.7$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation C

$C_6H_5NO_3$ (c) 72BOO/HAU
4-Nitrophenol
Phase Changes
c/liq 368.75 K, $\Delta H = 19300$ J·mol^{-1}
$\Delta S = 52.3$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation C

$C_6H_5NO_3$ (c) 82POE/FAN
4-Nitrophenol
Phase Changes
c/liq 387.0 K, $\Delta H = 18254$ J·mol^{-1}
$\Delta S = 47.17$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation A

$C_6H_5NO_3$ (c) 86SIN/KUM
4-Nitrophenol
Phase Changes
c/liq 385.15 K, $\Delta H = 30118$ J·mol^{-1}
$\Delta S = 78.2$ J·mol^{-1}·K^{-1}
Molecular Weight 139.1104
Wiswesser Line Notation WNR DQ
Evaluation A

$C_6H_5N_3$ (c) 89JIM/ROU
Benzotriazole
Heat Capacity 298.15 K, $C_p = 178.7$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 119.1256
Wiswesser Line Notation T56 BMNNJ
Evaluation A

C_6H_6 (c) 82BAT/MRA
2,4-Hexadiyne
Heat Capacity 298.15 K, C_p = 133.57 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 178.14 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 117.9 K, ΔH = 996.6 J·mol^{-1}
ΔS = 8.42 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation 2UU2UU2
Evaluation A

C_6H_6 (liq) 65FIN/GRU
Benzene
Heat Capacity 300 K, C_p = 135.30 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 69SUB/KHA
Benzene
Heat Capacity 298 K, C_p = 135.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 74RAJ/SUB
Benzene
Heat Capacity 298.15 K, C_p = 135.7 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 323.15 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 76FOR/BEN2
Benzene
Heat Capacity 298.15 K, C_p = 135.760 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A
Data from 76FOR/BEN.

C_6H_6 (liq) 77VES/SVO
Benzene
Heat Capacity 298.15 K, C_p = 135.90 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 79SMI
Benzene
Phase Changes
c/liq 279.1 K, ΔH = 9300 J·mol^{-1}
ΔS = 33.3 J·mol^{-1}·K^{-1}
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation C

C_6H_6 (liq) 82GOR/SIM2
Benzene
Heat Capacity
Temperature range 280 to 680 K.
Data at atmospheric pressure given by the equation:
$C_p = 1.5194 - 1.299\times10^{-3}T + 6.927\times10^{-6}T^2$ kJ·kg^{-1}·K^{-1}.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

C_6H_6 (liq) 83GOR/SIM
Benzene
Heat Capacity 298.15 K, C_p = 136.24 J·mol^{-1}·K^{-1}
Temperature range 283.78 to 348.47 K.
$C_p = 1.3943 - 5.857\times10^{-4}T + 5.89\times10^{-6}T^2$ kJ·kg^{-1}·K^{-1}.
C_p value calculated from equation.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 86RED
Benzene
Heat Capacity 303.15 K, C_p = 137.4 J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation B

C_6H_6 (liq) 88SHI/OGA
Benzene
Heat Capacity 298.15 K, C_p = 134.63 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 78.1134
Wiswesser Line Notation R
Evaluation A

$C_6H_6N_2O_2$ (c) 72BOO/HAU
3-Nitroaniline
Phase Changes
c/liq 384.95 K, ΔH = 23600 J·mol^{-1}
ΔS = 61.3 J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation C

$C_6H_6N_2O_2$ (c) 83NIS/SAK
3-Nitroaniline
Heat Capacity 298.15 K, C_p = 158.84 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.15 J·K^{-1}·g^{-1}.
Molecular Weight 138.1256
Wiswesser Line Notation ZR CNW
Evaluation B

$C_6H_6N_2O_2$ (c) 72BOO/HAU
4-Nitroaniline
Phase Changes
c/liq 420.65 K, ΔH = 21150 J·mol^{-1}
ΔS = 50.3 J·mol^{-1}·K^{-1}
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation C

$C_6H_6N_2O_2$ (c) 83NIS/SAK
4-Nitroaniline
Heat Capacity 298.15 K, C_p = 154.2 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 1.116 J·K^{-1}·g^{-1}.
Molecular Weight 138.1256
Wiswesser Line Notation ZR DNW
Evaluation B

C_6H_6O (c) 1889EYK
Phenol
Phase Changes
c/liq 312.7 K, ΔH = 10581 J·mol^{-1}
ΔS = 33.8 J·mol^{-1}·K^{-1}
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation C

C_6H_6O (liq) 03MAG
Phenol
Heat Capacity 298 K, C_p = 220.9 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.561 cal·g^{-1}·K^{-1}.
Molecular Weight 94.1128
Wiswesser Line Notation QR
Evaluation D

$C_6H_6O_2$ (c) 03MAG
1,2-Dihydroxybenzene; Pyrocatechin; Catechol
Heat Capacity 298 K, C_p = 144.2 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.313 cal·g^{-1}·K^{-1}.
Molecular Weight 110.1122
Wiswesser Line Notation QR BQ
Evaluation D

$C_6H_6O_2$ (c) 03MAG
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Heat Capacity 298 K, C_p = 122.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.266 cal·g^{-1}·K^{-1}.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation D

$C_6H_6O_2$ (c) 82VII/GAM
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Phase Changes
c/liq 381 K, ΔH = 20500 J·mol^{-1}
ΔS = 53.8 J·mol^{-1}·K^{-1}
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation B

$C_6H_6O_2$ (c) 87EBI/ASK
1,3-Dihydroxybenzene; Resorcin; Resorcinol
Phase Changes
c,II/c,I 369 K, ΔH = 1370 J·mol^{-1}
ΔS = 3.71 J·mol^{-1}·K^{-1}
α-β phase transition.
c,I/liq 382.7 K, ΔH = 20890 J·mol^{-1}
ΔS = 54.59 J·mol^{-1}·K^{-1}
Fusion of β-resorcinol.
Molecular Weight 110.1122
Wiswesser Line Notation QR CQ
Evaluation A

$C_6H_6O_2$ (c) 03MAG
1,4-Dihydroxybenzene; Hydroquinone
Heat Capacity 298 K, C_p = 118.9 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.258 cal·g^{-1}·K^{-1}.
Molecular Weight 110.1122
Wiswesser Line Notation QR DQ
Evaluation D

C_6H_7N (liq) 01KAH
2-Methylpyridine; α-Picoline
Heat Capacity C_p = 169.2 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K.
Heat capacity is an average value over the temperature range.
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ B1
Evaluation D

C_6H_7N (liq) 86STE/CHI
4-Methylpyridine
Heat Capacity 298.15 K, C_p = 158.99 J·mol^{-1}·K^{-1}
Temperature range 10 to 410 K.
Entropy 298.15 K, S = 208.22 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.010 K
c,I/liq 276.818 K
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ D1
Evaluation A

C_6H_7N (liq) 87MES/TOD
4-Methylpyridine
Heat Capacity 298.15 K, C_p = 158.99 J·mol^{-1}·K^{-1}
Temperature range 10 to 410 K.
Entropy 298.15 K, S = 208.22 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.010 K, ΔH = 0.083 J·mol^{-1}
c,I/liq 276.817 K, ΔH = 12577 J·mol^{-1}
ΔS = 45.43 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ D1
Evaluation A

C_6H_7N (liq) 88MES/TOD
4-Methylpyridine
Heat Capacity 298.150 K, C_p = 158.988 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S = 209.091 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 255.00 K, ΔH = 0.00 J·mol^{-1}
c,I/liq 276.818 K, ΔH = 12582.28 J·mol^{-1}
ΔS = 45.45 J·mol^{-1}·K^{-1}
Molecular Weight 93.1280
Wiswesser Line Notation T6NJ D1
Evaluation A

C_6H_7N (liq) 87LES/LIC
Aniline
Heat Capacity 298 K, C_p = 194.1 J·mol^{-1}·K^{-1}
Temperature range 200 to 300 K.
Phase Changes
c/liq 267 K
Molecular Weight 93.1280
Wiswesser Line Notation ZR
Evaluation B

C_6H_7N·HBr (c) 78KOJ
Aniline hydrobromide
Heat Capacity
Temperature range 200 to 320 K.
Data given graphically.
Phase Changes
c,II/c,I 230–300 K, ΔH = 1142 J·mol^{-1}
ΔS = 3.87 J·mol^{-1}·K^{-1}
Peak at 295 K for order-disorder transition which extends over a 70 K range (230–300 K).
Molecular Weight 174.0399
Wiswesser Line Notation ZR &EH
Evaluation B

$C_6H_8N_2$ (liq) 81LEB/RYA
Phenylhydrazine
Heat Capacity 299.45 K, C_p = 217.3 J·mol^{-1}·K^{-1}
Temperature range 293 to 358 K.
Molecular Weight 108.1426
Wiswesser Line Notation ZMR
Evaluation B

$C_6H_8N_2$ (c) 84RAB/KAR
1,3-Phenylenediamine
Heat Capacity 298.15 K, C_p = 159.6 J·mol^{-1}·K^{-1}
Temperature range 13 to 500 K.
Entropy 298.15 K, S = 154.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 339.1 K, ΔH = 15570 J·mol^{-1}
ΔS = 45.92 J·mol^{-1}·K^{-1}
Molecular Weight 108.1426
Wiswesser Line Notation ZR CZ
Evaluation A

$C_6H_8N_2$ (liq) 87LES/LIC
1,3-Phenylenediamine
Heat Capacity 298 K, C_p = 153.7 J·mol^{-1}·K^{-1}
Temperature range 220 to 400 K.
Phase Changes
c/liq 337 K
Molecular Weight 108.1426
Wiswesser Line Notation ZR CZ
Evaluation B

$C_6H_8N_2O_2$ (c) 84ZIE/ZIE
1,3-Dimethyluracil
Phase Changes
c/liq 392.5 K, ΔH = 23100 J·mol^{-1}
ΔS = 58.9 J·mol^{-1}·K^{-1}
Molecular Weight 140.1414
Wiswesser Line Notation T6NVNVJ A1 C1
Evaluation B

$(C_6H_8N_2O_9)_n$ (c) 85RAB/KHL
Cellulose nitrate
Heat Capacity 298.15 K, C_p = 279.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Entropy 298.15 K, S = 318.9 J·mol^{-1}·K^{-1}
Molecular Weight 252.1373
Wiswesser Line Notation /T5OTJ B* CONW DONW EO* FIQ/
Evaluation B
11.9% nitrogen content.
Dinitrocellulose has a nitrogen content of 11.11%.

$C_6H_8O_2$ (c) 83DEW/DEK
1,4-Cyclohexanedione
Heat Capacity 300 K, C_p = 161.4 J·mol^{-1}·K^{-1}
Temperature range 90 to 310 K.
Linearly extrapolated.
Phase Changes
c,III/c,II 319.89 K
c,II/c,I 336.73 K
c,I/liq 351.6 K, ΔH = 11325 J·mol^{-1}
Molecular Weight 112.1280
Wiswesser Line Notation L6V DVTJ
Evaluation B(C_p), A(Phase changes).

$C_6H_8O_4$ (c) 82LEB/KUL
Lactide(DL)
Heat Capacity 298.15 K, C_p = 184.3 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 213.1 J·mol^{-1}·K^{-1}
Molecular Weight 144.1268
Wiswesser Line Notation T6OV DOVTJ C1 F1
Evaluation A

$C_6H_8O_7$ (c) 82DEK/VAN
Citric acid
Heat Capacity 300 K, C_p = 226.51 J·mol^{-1}·K^{-1}
Temperature range 90 to 330 K.
Entropy 300 K, S = 252.1 J·mol^{-1}·K^{-1}
Molecular Weight 192.1250
Wiswesser Line Notation QV1XQVQ1VQ
Evaluation B(C_p), C(S)

$C_6H_9ClO_2$ (liq) 85KAR/ABD2
Chloroethyl methacrylate
Phase Changes
c/liq 235.1 K, ΔH = 17001 J·mol^{-1}
ΔS = 72.3 J·mol^{-1}·K^{-1}
Molecular Weight 148.5889
Wiswesser Line Notation G2OVY1&U1
Evaluation A

C_6H_9Cu (c) 81LEB/BYK
1-Hexynylcopper; Copper butylacetylenide
Heat Capacity 298.15 K, C_p = 160.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 180.6 J·mol^{-1}·K^{-1}
Molecular Weight 144.6831
Wiswesser Line Notation 5UU1-CU-
Evaluation A

C_6H_9Cu (c) 82BYK/LEB
1-Hexynylcopper; Copper butylacetylenide
Heat Capacity 298.15 K, C_p = 160.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 178.3 J·mol^{-1}·K^{-1}
Molecular Weight 144.6831
Wiswesser Line Notation 5UU1-CU-
Evaluation A

C_6H_9N (liq) 86STE/CHI
2,4-Dimethylpyrrole
Heat Capacity 298.15 K, C_p = 192.19 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 222.01 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 268.435 K
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 D1
Evaluation A

C_6H_9N (liq) 86STE/CHI
2,5-Dimethylpyrrole
Heat Capacity 298.15 K, C_p = 195.30 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 212.13 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 280.904 K
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 E1
Evaluation A

C_6H_9N (liq) 87MES/TOD
2,5-Dimethylpyrrole
Heat Capacity 298.15 K, C_p = 195.30 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 212.13 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 280.904 K, ΔH = 9296.0 J·mol^{-1}
ΔS = 33.09 J·mol^{-1}·K^{-1}
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 E1
Evaluation A

C_6H_9N (liq) 88MES/TOD
2,5-Dimethylpyrrole
Heat Capacity 298.150 K, C_p = 195.297 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S = 212.242 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 280.904 K, ΔH = 9298.42 J·mol^{-1}
ΔS = 33.10 J·mol^{-1}·K^{-1}
Molecular Weight 95.1438
Wiswesser Line Notation T5MJ B1 E1
Evaluation A

C_6H_{10} (liq) 88KAL/WOY
Cyclohexene
Heat Capacity 298.12 K, C_p = 152.90 J·mol^{-1}·K^{-1}
Temperature range 183 to 298 K.
Unsmoothed experimental datum.
Molecular Weight 82.1450
Wiswesser Line Notation L6UTJ
Evaluation B

$(C_6H_{10})_n$ (c) 88LEB/SMI
Ethylene-butadiene copolymer
Heat Capacity 298.15 K, C_p = 148.8 J·mol^{-1}·K^{-1}
Temperature range 30 to 330 K.
Entropy 298.15 K, S = 148.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 199 K
Glass transition.
c/liq 333 K
Molecular Weight 82.1450
Wiswesser Line Notation /*2*/ &/*1U2U1*/
Evaluation A

$C_6H_{10}N_2O$ (liq) 80BYS
2,3-Diazabicyclo[2.2.2]oct-2-ene N-oxide
Phase Changes
c,III/c,II 359.2 K, ΔH = 5020 J·mol^{-1}
ΔS = 14.0 J·mol^{-1}·K^{-1}
c,II/c,I 399.3 K, ΔH = 8050 J·mol^{-1}
ΔS = 20.2 J·mol^{-1}·K^{-1}
c,I/liq 437.9 K, ΔH = 3840 J·mol^{-1}
ΔS = 8.77 J·mol^{-1}·K^{-1}
Molecular Weight 126.1582
Wiswesser Line Notation T66 A B DNUNTJ DUO
Evaluation A

$C_6H_{10}O$ (liq) 80NAK/SUG
Cyclohexanone
Heat Capacity 300 K, C_p = 177.20 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Unsmoothed experimental datum for C_p at 296.40 K is 175.96 J·mol^{-1}·K^{-1}.
Entropy 300 K, S = 229.03 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 220.83 K, ΔH = 8659.6 J·mol^{-1}
ΔS = 39.22 J·mol^{-1}·K^{-1}
c,I/liq 245.21 K, ΔH = 1327.6 J·mol^{-1}
ΔS = 5.414 J·mol^{-1}·K^{-1}
Molecular Weight 98.1444
Wiswesser Line Notation L6VTJ
Evaluation A

$C_6H_{10}O$ (liq) 80NAK/SUG
Cyclohexene oxide
Heat Capacity 300 K, C_p = 166.12 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Unsmoothed experimental datum for C_p at 296.96 K is 164.98 J·mol^{-1}·K^{-1}.
Entropy 300 K, S = 221.98 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 193.10 K, ΔH = 9535.1 J·mol^{-1}
ΔS = 49.39 J·mol^{-1}·K^{-1}
c,I/liq 238.14 K, ΔH = 1064.5 J·mol^{-1}
ΔS = 4.470 J·mol^{-1}·K^{-1}
Molecular Weight 98.1444
Wiswesser Line Notation T36 BOTJ
Evaluation A

$C_6H_{10}O_2$ (liq) 82VIL/CAS
3,6-Dioxaoctane
Heat Capacity 298.15 K, C_p = 261.08 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.1438
Wiswesser Line Notation 20202
Evaluation B

$C_6H_{10}O_2$ (liq) 78LEB/YEV2
ϵ-Caprolactone
Heat Capacity 298.15 K, C_p = 196.8 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 350 K.
Entropy 298.15 K, S = 235.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 271.83 K, ΔH = 13820 J·mol^{-1}
ΔS = 50.9 J·mol^{-1}·K^{-1}
Molecular Weight 114.1438
Wiswesser Line Notation T7OVTJ
Evaluation A

$C_6H_{10}O_2$ (liq) 83LEB/YEV
ϵ-Caprolactone
Heat Capacity 298.15 K, C_p = 196.8 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 340 K.
Entropy 298.15 K, S = 235.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 272.13 K, ΔH = 13820 J·mol^{-1}
ΔS = 50.9 J·mol^{-1}·K^{-1}
Molecular Weight 114.1438
Wiswesser Line Notation T7OVTJ
Evaluation A

$(C_6H_{10}O_2)_n$ (c) 78LEB/YEV2
Poly-ϵ-caprolactone
Heat Capacity 298.15 K, C_p = 161.6 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 350 K.
Entropy 298.15 K, S = 181.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 336 K, ΔH = 16400 J·mol^{-1}
ΔS = 48.0 J·mol^{-1}·K^{-1}
Molecular Weight 114.1438
Wiswesser Line Notation /*OV5*/
Evaluation A
T(glass) = 209 K.

$C_6H_{10}O_4$ (liq) 83SAN/CIO
Ethylene glycol diacetate
Heat Capacity 298.15 K C_p = 310 J·mol^{-1}·K^{-1}
Temperature Range 273.15 to 323.15 K
C_p°(kJ kg^{-1}K^{-1}) = 0.044175T - 11.049
Molecular Weight 146.1426
Wiswesser Line Notation 1VO2OV1
Evaluation D

$C_6H_{10}O_4$ (liq) 86NIL/WAD
Ethyleneglycoldiacetate
Heat Capacity 298.15 K, C_p = 269.2 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 146.1426
Wiswesser Line Notation 1VO2OV1
Evaluation A

$C_6H_{10}O_4$ (c) 84VAS/PET
1,4-Butanedioic acid
Heat Capacity 298.15 K, C_p = 196.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 450 K.
Entropy 298.15 K, S = 219.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 424.7 K
Molecular Weight 146.1426
Wiswesser Line Notation QV4VQ
Evaluation A

$C_6H_8O_7{\cdot}H_2O$ (c) 82DEK/VAN
Citric acid monohydrate
Heat Capacity 300 K, C_p = 269.52 J·mol^{-1}·K^{-1}
Temperature range 120 to 300 K.
Entropy 300 K, S = 285.32 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 312.1 K, ΔH = 14980 J·mol^{-1}
ΔS = 48.0 J·mol^{-1}·K^{-1}
Molecular Weight 210.1402
Wiswesser Line Notation QV1XQVQ1VQ &QH
Evaluation B

$C_6H_{11}LiO_2$ (c) 86NGE/WES
Lithium n-hexanoate
Heat Capacity 298.15 K, C_p = 216.01 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 228.48 J·mol^{-1}·K^{-1}
Molecular Weight 122.0927
Wiswesser Line Notation OV5 .LI
Evaluation A

$C_6H_{11}NO$ (c) 62KOL/PAU
ϵ-Caprolactam
Heat Capacity 300.00 K, C_p = 156.3 J·mol^{-1}·K^{-1}
Temperature Range 60 to 350 K
Entropy 298.15 K, S = 168.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 342.305 K, ΔH = 16096 J·mol^{-1}
ΔS = 47.0 J·mol^{-1}·K^{-1}
Molecular Weight 113.1567
Wiswesser Line Notation T7MVTJ
Evaluation B

$(C_6H_{11}NO)_n$ (c) 62KOL/PAU
Poly-ϵ-caprolactam
Heat Capacity 298.15 K, C_p = 169.7 J·mol^{-1}·K^{-1}
Temperature Range 60 to 350 K
Entropy 298.15 K, S = 173.0 J·mol^{-1}·K^{-1}
Molecular Weight 113.1567
Wiswesser Line Notation /*MV4*/
Evaluation B

$C_6H_{11}NO_2$ (liq) 83GEI/KAR
1,1-Dimethoxy-3-cyanopropane; Dimethyl acetal of β-cyanopropionaldehyde
Heat Capacity 298.15 K, C_p = 253.63 J·mol^{-1}·K^{-1}
Temperature range 55 to 300 K.
Entropy 298.15 K, S = 295.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 154 K
Glassy (solid) to liquid transition.
Molecular Weight 129.1584
Wiswesser Line Notation NC2YO1&O1
Evaluation A

$C_6H_{11}O_2Tl$ (c) 76MEI/SEY
Thallium hexanoate
Phase Changes
c,III/c,II 395 K, ΔH = 179 J·mol^{-1}
ΔS = 0.46 J·mol^{-1}·K^{-1}
c,II/c,I 412 K, ΔH = 1841 J·mol^{-1}
ΔS = 1.84 J·mol^{-1}·K^{-1}
c,I/liq 418 K, ΔH = 4477 J·mol^{-1}
ΔS = 10.9 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 500 K, ΔH = 3035 J·mol^{-1}
ΔS = 6.69 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 319.5217
Wiswesser Line Notation OV5 .TL
Evaluation B

$C_6H_{11}O_2Tl$ (c) 84FER/LOP
Thallium hexanoate
Heat Capacity 320 K, C_p = 235 J·mol^{-1}·K^{-1}
Temperature range 320 to 480 K.
Phase Changes
c,III/c,II 397.9 K, ΔH = 208 J·mol^{-1}
ΔS = 0.50 J·mol^{-1}·K^{-1}
c,II/c,I 415.0 K, ΔH = 657 J·mol^{-1}
ΔS = 1.58 J·mol^{-1}·K^{-1}
c,I/liq 425.0 K, ΔH = 4598 J·mol^{-1}
ΔS = 10.8 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 319.5217
Wiswesser Line Notation OV5 .TL
Evaluation A
Mesophase to isotropic liquid phase change data also given:
499.8 K; ΔH = 3941 J·mol^{-1};
ΔS = 7.90 J·mol^{-1}·K^{-1}.

$C_6H_{11}O_2Tl$ (c) 85BOE/LOP
Thallium hexanoate
Heat Capacity 298.15 K, C_p = 234.96 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 324.76 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 203.5 K, ΔH = 1734 J·mol^{-1}
ΔS = 8.62 J·mol^{-1}·K^{-1}
c,IV/c,III 280.3 K, ΔH = 2511 J·mol^{-1}
ΔS = 8.88 J·mol^{-1}·K^{-1}
c,III/c,II 397.9 K
c,II/c,I 415.0 K
c,I/liq 425.0 K
Solid-mesomorphic liquid.
Molecular Weight 319.5217
Wiswesser Line Notation OV5 .TL
Evaluation A
Mesomorphic liquid-isotropic liquid transition at 499.8 K.
See 84FER/LOP, 81LIN/DIE, and 76MEI/SEY for transition data.

C_6H_{12} (liq) 85KAL/WOY
1-Hexene
Heat Capacity 298.56 K, C_p = 182.77 J·mol^{-1}·K^{-1}
Temperature range 180 to 300 K.
Value is unsmoothed experimental datum.
Molecular Weight 84.1608
Wiswesser Line Notation 5U1
Evaluation B

C_6H_{12} (liq) 50AUE/SAG
Cyclohexane
Heat Capacity 300 K, C_p = 154.2 J·mol^{-1}·K^{-1}
Temperature range 300 to 366 K;
C_p given as 0.4378 Btu(lb)$^{-1}$(°R)$^{-1}$ at 80°F.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 76FOR/BEN2
Cyclohexane
Heat Capacity 298.15 K, C_p = 156.070 J·mol^{-1}·K^{-1}
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A
Data from 76FOR/BEN.

C_6H_{12} (liq) 77VES/SVO
Cyclohexane
Heat Capacity 298.15 K, C_p = 156.12 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 78SAF
Cyclohexane
Heat Capacity 298 K, C_p = 156.7 J·mol^{-1}·K^{-1}
Temperature range 298 to 313 K.
Data calculated from equation
$C_p = 1.7493 + 0.00452\,T$ kJ·kg^{-1}·K^{-1}.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 86JIM/ROM
Cyclohexane
Heat Capacity 298.15 K, C_p = 157.06 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation B

C_6H_{12} (liq) 88SHI/OGA2
Cyclohexane
Heat Capacity 298.15 K, C_p = 154.32 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 84.1608
Wiswesser Line Notation L6TJ
Evaluation A

$(C_6H_{12})_n$ (gls) 74LEB/LEB
1-Polyhexene
Entropy 298.15 K, S = 171.3 J·mol^{-1}·K^{-1}
Deposited in VINITI, No 2118-74, 30 July 1974.
Molecular Weight 84.1608
Wiswesser Line Notation /*Y4&1*/
Evaluation A
T(glass) = 215.5 K.

$C_6H_{12}BNO_3$ (c) 64CAS/STO
Triethanolamine borate
Heat Capacity 298.15 K, C_p = 187.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 183.2 J·mol^{-1}·K^{-1}
Molecular Weight 156.9757
Wiswesser Line Notation T88 A B C AO DN GO HB IOTJ
Evaluation A

$C_6H_{12}BNO_3$ (c) 64CLE/WON
Triethanolamine borate
Heat Capacity 320 K, C_p = 226.4 J·mol^{-1}·K^{-1}
Temperature range 320 to 525 K.
Entropy 320 K, S = 216.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 466.54 K, ΔH = 4774 J·mol^{-1}
ΔS = 10.3 J·mol^{-1}·K^{-1}
c,I/liq 511.86 K, ΔH = 24100 J·mol^{-1}
ΔS = 47.11 J·mol^{-1}·K^{-1}
Molecular Weight 156.9757
Wiswesser Line Notation T88 A B C AO DN GO HB IOTJ
Evaluation A

$C_6H_{12}BrFeN_2S_4$ 89YOS/SOR
Bis(N,N-Dimethyldithiocarbamato) iron (III) bromide
Heat Capacity 296.421 K C_p = 294.9 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K;
C_p value is unsmoothed experimental datum.
Phase Changes
c,III/c,II 0.837 K
Ferromagnetic/paramagnetic transition
c,II/c,I 8.8 K ΔH = 5.77 J·mol^{-1}
ΔS = 6.05 J·mol^{-1}·K^{-1}
Schottky anomaly
Molecular Weight 376.1898
Wiswesser Line Notation SUYS&N1&1 2 .FE &E
Evaluation A
The total magnetic entropy and enthalpy in the temperature range 0.4 to 30 K are S = 11.74 J·mol^{-1}·K^{-1} and 92.0 J·mol^{-1}, respectively.

$C_6H_{12}ClFeN_2S_4$ (c) 84YOS/SOR
Chlorobis(N,N-dimethyldithiocarbamate)iron(III)
Heat Capacity 300 K, C_p = 299 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K.
Data graphically only.
Value estimated from graph.
Phase Changes
c,III/c,II 0.609 K
Lambda transition.
c,II/c,I 2 K
Schottky-type anomaly.
Molecular Weight 331.7142
Wiswesser Line Notation SUYS&N1&1 2 .FE &G
Evaluation A
Total magnetic entropy is 14.05 J·mol^{-1}·K^{-1}.

$C_6H_{12}Cl_2$ (liq) 85LAI/GRO
1,6-Dichlorohexane
Heat Capacity 298.15 K, C_p = 239.57 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 155.0668
Wiswesser Line Notation G6G
Evaluation B

$C_6H_{12}FeIN_2S_4$ (c) 83YOS/SOR2
Iodobis(N,N-dimethyldithiocarbamato) iron (III)
Heat Capacity 298.352 K, C_p = 301.9 J·mol^{-1}·K^{-1}
Temperature range 0.4 to 300 K.
Unsmoothed experimental datum.
Molecular Weight 423.1657
Wiswesser Line Notation SYUS&N1&1 2 .FE &I
Evaluation A
Lambda type anomaly observed at 1.65 K;
Schottky type anomaly observed at ca. 0.7 K.

$C_6H_{12}O$ (liq) 70HAR/HEA
3,3-Dimethyl-2-butanone; Methyl *tert*-butyl ketone
Heat Capacity 298.15 K, C_p = 207.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation 1X1&1&V1
Evaluation B

$C_6H_{12}O$ (liq) 89VES/BAR
4-Methyl-2-pentanone; Isobutyl methyl ketone
Heat Capacity 298.15 K C_p = 211.9 J·mol^{-1}·K^{-1}
Molecular Weight 100.1602
Wiswesser Line Notation 1Y1&1V1
Evaluation A

$C_6H_{12}O$ (liq) 70HAR/HEA
3-Hexanone; Ethyl *n*-propyl ketone
Heat Capacity 298.15 K, C_p = 216.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation 3V2
Evaluation B

$C_6H_{12}O$ (liq) 70HAR/HEA
2-Hexanone; Methyl *n*-butyl ketone
Heat Capacity 298.15 K, C_p = 213.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.1602
Wiswesser Line Notation 4V1
Evaluation B

$C_6H_{12}O_2$ (liq) 86JIM/ROM
Propyl propionate; *n*-Propyl propanoate
Heat Capacity 298.15 K, C_p = 226.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 3OV2
Evaluation B

$C_6H_{12}O_2$ (liq) 87ZAB/HYN
Propyl propionate; *n*-Propyl propanoate
Heat Capacity 298.38 K, C_p = 229.00 J·mol^{-1}·K^{-1}
Temperature range 294 to 367 K.
Unsmoothed experimental datum.
Molecular Weight 116.1596
Wiswesser Line Notation 3OV2
Evaluation B

$C_6H_{12}O_2$ (liq) 86JIM/ROM
n-Butyl acetate; *n*-Butyl ethanoate
Heat Capacity 298.15 K, C_p = 225.11 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.1596
Wiswesser Line Notation 4OV1
Evaluation B

$C_6H_{12}O_2$ (liq) 87ZAB/HYN
n-Butyl acetate; *n*-Butyl ethanoate
Heat Capacity 298.35 K, C_p = 228.11 J·mol^{-1}·K^{-1}
Temperature range 294 to 364 K.
Unsmoothed experimental datum.
Molecular Weight 116.1596
Wiswesser Line Notation 4OV1
Evaluation B

$C_6H_{12}O_3$ (liq) 83SAN/CIO
2-Ethoxyethanol acetate
Heat Capacity 298.15 K, C_p = 376 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K.
$C_p°$(kJ·kg^{-1}K^{-1}) = 0.009426T + 0.036
Molecular Weight 132.1590
Wiswewesser Line Notation 1VO2O2
Evaluation D

$C_6H_{12}O_6$ (c) 82LIA/CHE
meso-Inositol
Heat Capacity 298.15 K, C_p = 218.31 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 180.1572
Wiswesser Line Notation L6TJ AQ BQ CQ DQ EQ FQ
Evaluation B

$C_6H_{12}O_6$ (c) 03MAG
Fructose
Heat Capacity 298 K, C_p = 208.0 J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.276 cal·g^{-1}·K^{-1}.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ B1Q CQ DQ EQ
A&DE -B&BC
Evaluation D

$C_6H_{12}O_6$ (c) 81KAW/KUS
Fructose(D)
Heat Capacity 303 K, C_p = 232 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ B1Q CQ DQ EQ −A&DE −B&BC
Evaluation B

$C_6H_{12}O_6$ (c) 81KAW/KUS
Mannose(D)
Heat Capacity 303 K, C_p = 216 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q −A&E −B&CDF
Evaluation B

$C_6H_{12}O_6$ (c) 81KAW/KUS
Galactose(D)
Heat Capacity 303 K, C_p = 217 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q −A&BC −B&DEF
Evaluation B

$C_6H_{12}O_6$ (c) 03MAG
α-Glucose(D)
Heat Capacity 298 K, C_p = 235.9 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.313 cal·g^{-1}·K^{-1}.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q −A&BCE −B&DF
Evaluation D

$C_6H_{12}O_6$ (c) 81KAW/KUS
α-Glucose(D)
Heat Capacity 303 K, C_p = 224 J·mol^{-1}·K^{-1}
Temperature range 300 to 315 K.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q −A&BCE −B&DF
Evaluation B

$C_6H_{12}O_6$ (c) 82LIA/CHE
α-Glucose(D)
Heat Capacity 298.15 K, C_p = 219.79 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 180.1572
Wiswesser Line Notation T6OTJ BQ CQ DQ EQ F1Q −A&BCE −B&DF
Evaluation B

$C_6H_{13}N$ (liq) 86STE/CHI
2-Methylpiperidine
Heat Capacity 298.15 K, C_p = 212.97 J·mol^{-1}·K^{-1}
Temperature range 10 to 380 K.
Entropy 298.15 K, S = 243.75 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.357 K
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation A

$C_6H_{13}N$ (liq) 87MES/TOD
2-Methylpiperidine
Heat Capacity 298.15 K, C_p = 212.96 J·mol^{-1}·K^{-1}
Temperature range 10 to 390 K.
Entropy 298.15 K, S = 243.75 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.357 K, ΔH = 18583.6 J·mol^{-1}
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation A

$C_6H_{13}N$ (liq) 88MES/TOD
2-Methylpiperidine
Heat Capacity 298.150 K, C_p = 212.965 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S = 243.762 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.357 K, ΔH = 18583.87 J·mol^{-1}
Molecular Weight 99.1754
Wiswesser Line Notation T6MTJ B1
Evaluation A

$C_6H_{13}NO$ (liq) 76SKO/SUU
N-Methylpentanamide; N-Methylvaleramide
Heat Capacity 298.15 K, C_p = 238.4 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 115.1748
Wiswesser Line Notation 4VM1
Evaluation A

$C_6H_{13}NO_2$ (c) 84GRU/BOU
Leucine (L); 2-Amino-4-methylpentanoic acid (L)
Phase Changes
c,II/c,I 352 K, ΔH = 200 J·mol^{-1}
ΔS = 0.57 J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ1Y1&1−L
Evaluation B

$C_6H_{13}NO_2$ (c) 84GRU/BOU
Norleucine (L); α-Aminocaproic acid (L)
Phase Changes
c,II/c,I 389 K, ΔH = 110 J·mol^{-1}
ΔS = 0.28 J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ4 -L
Evaluation B

$C_6H_{13}NO_2$ (c) 84GRU/BOU
Norleucine (DL); α-Aminocaproic acid (DL)
Phase Changes
c,II/c,I 390 K, ΔH = 4410 J·mol^{-1}
ΔS = 11.31 J·mol^{-1}·K^{-1}
Molecular Weight 131.1742
Wiswesser Line Notation QVYZ4
Evaluation B

$C_6H_{13}NO_2$ (c) 83SKO/SAB
6-Aminohexanoic acid
Heat Capacity 298 K, C_p = 175.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 131.1742
Wiswesser Line Notation Z5VQ
Evaluation B

$C_6H_{14}O_6$ (c) 82LIA/CHE
Sorbitol(D)
Heat Capacity 298.15 K, C_p = 241.43 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQ 2−BBAA
Evaluation B

$C_6H_{14}O_6$ (c) 03MAG
Mannitol
Heat Capacity 298 K, C_p = 240.1 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.315 cal·g^{-1}·K^{-1}.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q−DDLL
Evaluation D

$C_6H_{14}O_6$ (c) 82LIA/CHE
Mannitol(D)
Heat Capacity 298.15 K, C_p = 239.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q−DDLL−D
Evaluation B

$C_6H_{14}O_6$ (c) 03MAG
Dulcite; Dulcitol; Galactitol
Heat Capacity 298 K, C_p = 215.7 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.283 cal·g^{-1}·K^{-1}.
Molecular Weight 182.1730
Wiswesser Line Notation Q1YQYQYQYQ1Q−DLLD
Evaluation D

$C_6H_{14}S$ (liq) 82TUT/GAB
1-Hexanethiol; *n*-Hexyl mercaptan
Heat Capacity 300 K, C_p = 237.90 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 221.21 + 3.060\times10^{-2}T + 8.343\times10^{-5}T^2$.
Molecular Weight 118.2366
Wiswesser Line Notation SH6
Evaluation B

$C_6H_{15}Al$ (liq) 84SHE/NIS
Triethylaluminum
Heat Capacity 298.15 K, C_p = 239.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 307.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.00 K, ΔH = 10600 J·mol^{-1}
ΔS = 47.11 J·mol^{-1}·K^{-1}
Molecular Weight 114.1660
Wiswesser Line Notation 2-AL-2&2
Evaluation A

$C_6H_{15}Al$ (liq) 89RAB/NIS
Triethylaluminum
Heat Capacity 298.15 K, C_p = 239.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 313 K.
Entropy 298.15 K, S = 308.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 225.00 K, ΔH = 10600 J·mol^{-1}
ΔS = 47.11 J·mol^{-1}·K^{-1}
Molecular Weight 114.1660
Wiswesser Line Notation 2-AL-2&2
Evaluation A

$C_6H_{15}B$ (c) 77KOS/SAM
Triethylboron
Heat Capacity 298.15 K, C_p = 240 J·mol^{-1}·K^{-1}
Temperature range 12 to 322 K.
Data calculated from equation.
$C_p = 6.2328 + 0.17161\ T$ cal·mol^{-1}·K^{-1}.
Entropy 298.15 K, S = 330.05 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 180.21 K, ΔH = 11522 J·mol^{-1}
ΔS = 63.94 J·mol^{-1}·K^{-1}
liq/g 321.81 K
Molecular Weight 97.9945
Wiswesser Line Notation 2B2&2
Evaluation B

$C_6H_{15}N$ (liq) 01KAH
Dipropylamine
Heat Capacity C_p = 252.6 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K.
Heat capacity is an average value over the temperature range.
Molecular Weight 101.1912
Wiswesser Line Notation 3M3
Evaluation D

$C_6H_{15}N_3$ (liq) 88BOB/KAM
N-(2-Aminoethyl)piperazine
Heat Capacity 333 K, C_p = 284 J·mol^{-1}·K^{-1}
Temperature Range 333 to 473 K
Molecular Weight 129.2046
Wiswesser Line Notation T6M DNTJ D2Z
Evaluation D

$C_6H_{15}NO_3$ (liq) 82MIN/SAB
Triethanolamine
Heat Capacity 298.15 K, C_p = 389 J·mol^{-1}·K^{-1}
One temperature. C_p given as 2.6 J·K^{-1}·g^{-1}.
Molecular Weight 149.1894
Wiswesser Line Notation Q2N2Q2Q
Evaluation C

$C_6H_{16}Si_2$ (c) 75GUS/KAR
1,1,3,3-Tetramethyl-1,3-disilacyclobutane
Heat Capacity 298.15 K, C_p = 216.94 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Data given graphically.
Entropy 298.15 K, S = 296.27 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 266.02 K, ΔH = 10259 J·mol^{-1}
ΔS = 38.58 J·mol^{-1}·K^{-1}
liq/g 390.93 K, ΔH = 39480 J·mol^{-1}
ΔS = 91.34 J·mol^{-1}·K^{-1}
Molecular Weight 144.3634
Wiswesser Line Notation T4-SI-TJ A1 A1 C_1 C1
Evaluation B

$C_6H_{17}BeF_4N_3O_6$ (c) 79LOI/OSB
Triglycine fluoroberyllate
Heat Capacity 300 K, C_p = 412.8 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K.
C_p given as 0.316 cal·g^{-1}·K^{-1}.
Molecular Weight 312.2226
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4
Evaluation B

$C_6H_{17}BeF_4N_3O_6$ (c) 81LOI/KOS
Triglycine fluoroberyllate
Heat Capacity 308 K, C_p = 444 J·mol^{-1}·K^{-1}
One temperature.
C_p(35 °C) = 0.34 cal·g^{-1}· °C^{-1}.
Molecular Weight 312.2226
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4
Evaluation B

$C_6H_{17}BeF_4N_3O_6$ (c) 81LOI/KOS2
Triglycine fluoroberyllate
Phase Changes
c,II/c,I 345 K, ΔH = 1254 J·mol^{-1}
ΔS = 3.63 J·mol^{-1}·K^{-1}
Ferroelectric transition.
Molecular Weight 312.2226
Wiswesser Line Notation Z1VQ 3 &H2 .BE F4
Evaluation C

$C_6H_{17}N_3O_{10}S$ (c) 75CAM/GON
Triglycine sulfate
Heat Capacity 300 K, C_p = 420 J·mol^{-1}·K^{-1}
Temperature range 100 to 400 K.
Data given graphically; C_p estimated from graph.
Phase Changes
c,II/c,I 322.55 K, ΔH = 614 J·mol^{-1}
ΔS = 1.9 J·mol^{-1}·K^{-1}
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation C_p(D); Phase change(B)

$C_6H_{17}N_3O_{10}S$ (c) 79LOI/OSB
Triglycine sulfate
Heat Capacity 300 K, C_p = 407 J·mol^{-1}·K^{-1}
Temperature range 294 to 340 K. C_p=0.301 cal·g^{-1}·K^{-1}.
Phase Changes
c,II/c,I ΔH = 622 J·mol^{-1}
No temperature given.
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation B

$C_6H_{17}N_3O_{10}S$ (c) 81LOI/KOS
Triglycine sulfate
Heat Capacity 308 K, C_p = 419 J·mol^{-1}·K^{-1}
One temperature.
C_p(35 °C) = 0.31 cal·g^{-1}· °C^{-1}.
Molecular Weight 323.2804
Wiswesser Line Notation Z1VQ 3 &WSQQ
Evaluation B

$C_6H_{17}N_3O_{10}S$·$C_6H_{17}N_3O_{10}Se$ (c) 83GUL/POL
Triglycine sulfate-triglycine selenate
Heat Capacity 303 K, C_p = 461 J·mol^{-1}·K^{-1}
One temperature. C_p = 1.26 J·g^{-1}·C^{-1}.
Molecular Weight 365.4850
Wiswesser Line Notation Z1VQ 3 &WSQQ – &Z1VQ 3 &W-SE-QQ
Evaluation C
$TGS_{0.10}$– $TGSe_{0.90}$

$C_6H_{18}N_4$ (liq) 88BOB/KAM
Triethylenetetramine
Heat Capacity 333 K, C_p = 376 J·mol^{-1}·K^{-1}
Temperature Range 333 to 473 K
Molecular Weight 146.2350
Wiswesser Line Notation Z2M2M2Z
Evaluation D

$C_6H_{18}N_3OP$ (liq) 82VOR/YAK
Hexamethylphosphoramide; Hexamethylphosphoric triamide
Heat Capacity 298.15 K, C_p = 321.3 J·mol^{-1}·K^{-1}
Temperature range 297.15 to 299.15 K.
C_p given as 1.793 J·K^{-1}·g^{-1}.
Molecular Weight 179.2015
Wiswesser Line Notation OPN1&1&N1&1&N1&1
Evaluation B

$C_6H_{18}Si_2$ (liq) 59SUG/SEK
Hexamethyldisilane
Heat Capacity 295.67 K, C_p = 255.9 J·mol^{-1}·K^{-1}
Temperature range 206 to 296 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 221.8 K, ΔH = 9749 J·mol^{-1}
ΔS = 43.93 J·mol^{-1}·K^{-1}
c,I/liq 287.72 K, ΔH = 3017 J·mol^{-1}
ΔS = 10.50 J·mol^{-1}·K^{-1}
Molecular Weight 146.3792
Wiswesser Line Notation 1-SI-1&1-SI-1&1&1
Evaluation C

$C_6H_{20}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(propylammonium) manganese II
Phase Changes
c,IV/c,III 323 K, ΔH = 67.2 J·mol^{-1}
ΔS = 0.22 J·mol^{-1}·K^{-1}
c,III/c,II 383 K, ΔH = 14.4 J·mol^{-1}
ΔS = 0.036 J·mol^{-1}·K^{-1}
c,II/c,I 445 K, ΔH = 5.3 J·mol^{-1}
ΔS = 0.12 J·mol^{-1}·K^{-1}
Molecular Weight 316.9874
Wiswesser Line Notation 3ZH 2 .MN G4
Evaluation A

$C_6H_{21}N_3Si_3$ (liq) 81MEK/KAR
Hexamethyltrisilazane
Heat Capacity 298.15 K, C_p = 428.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Data given graphically.
Entropy 298.15 K, S = 460 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 254.4 K, ΔH = 15171 J·mol^{-1}
ΔS = 61.38 J·mol^{-1}·K^{-1}
Molecular Weight 219.5085
Wiswesser Line Notation T6-SI-M-SI-M-SI-MTJ A1 A1 C_1 C_1 E1 E1
Evaluation A

$C_6O_{12}Ce_2$ (c) 85GAL/DWO
Cerium(III) oxalate
Heat Capacity 418 K, C_p = 499.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 773 K.
$C_p = 3.2177\times10^{1} - (1.9668\times10^{-1})T + (4.0732\times10^{-4})T^2 - (2.7686\times10^{-7})T^3$ J·K^{-1}·g^{-1} over the temperature range 418 to 538 K.
Molecular Weight 544.2888
Wiswesser Line Notation OV1 3 .CE 2
Evaluation B

C_7F_{16} (liq) 51OLI/GRI
Perfluoroheptane; Hexadeca-fluoroheptane
Heat Capacity 300 K, C_p = 419.47 J·mol^{-1}·K^{-1}
Temperature range 18 to 310 K
Entropy 298.15 K, S = 561.80 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 180.45 K, ΔH = 6670.6 J·mol^{-1}
ΔS = 36.97 J·mol^{-1}·K^{-1}
c,I/liq 221.86 K, ΔH = 6947.2 J mol^{-1}
ΔS = 31.31 J·mol^{-1}·K^{-1}
Molecular Weight 388.0514
Wiswesser Line Notation FXFFXFFXFFXFFXFFXF FXFFF
Evaluation A

C_7F_{16} (liq) 83CAM/DIA
Perfluoroheptane; Hexadecafluoroheptane
Heat Capacity 293 K, C_p = 322.2 J·mol^{-1}·K^{-1}
Interpolated data.
Molecular Weight 388.0514
Wiswesser Line Notation FXFFXFFXFFXFFXFFXFFXFFF
Evaluation C

$C_7H_4CrO_3S$ (c) 78POM/CHH
Thiophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p = 193.0 J·mol^{-1}·K^{-1}
Temperature range 120 to 300 K.
Data given graphically.
$C_p = 71.02 - 4.41\times10^{-1}\,T + 4.61\times10^{-3}T^2 - 5.96\times10^{-6}T^3$ J·mol^{-1}·K^{-1}
(105 to 130 K; 245 to 300 K).
C_p value calculated from equation.
Phase Changes
c,II/c,I 185 K, ΔH = 1650 J·mol^{-1}
ΔS = 8.95 J·mol^{-1}·K^{-1}
Molecular Weight 220.1628
Wiswesser Line Notation T5SØJ Ø-CR-- CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4CrO_3Se$ (c) 78POM/CHH
Selenophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p = 272.9 J·mol^{-1}·K^{-1}
Temperature range 125 to 337 K.
Data given graphically.
$Sp = 116.8 + 2.69\times10^{-1}T + 1.48\times10^{-3}T^2 - 2.08\times10^{-6}T^3$ J·mol^{-1}·K^{-1} (125 to 337K).
C_p value calculated from equation.
Molecular Weight 267.0628
Wiswesser Line Notation T5-SE-ØJ Ø-CR-- CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4CrO_3Te$ (c) 78POM/CHH
Tellurophene chromium tricarbonyl
Heat Capacity 298.15 K, C_p = 278.7 J·mol^{-1}·K^{-1}
Temperature range 124 to 326 K.
Data given graphically.
$C_p = 96.85 + 1.67\times10^{-1}T + 2.44\times10^{-3}T^2 - 3.19\times10^{-6}T^3$ J·mol^{-1}·K^{-1} (124 to 326 K).
C_p value calculated from equation.
Molecular Weight 315.7028
Wiswesser Line Notation T5-TE-ØJ Ø-CR-- CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4F_3NO_2$ (liq) 81LEB/RYA
3-Trifluoromethyl nitrobenzene
Heat Capacity C_p = 224.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 373 K.
Heat capacity is an average value.
Data given over temperature range.
Molecular Weight 191.1093
Wiswesser Line Notation WNR CXFFF
Evaluation B

$C_7H_4MnNO_3$ (c) 78POM/CHH
Azacymantrene; Pyrroyl manganese tricarbonyl
Heat Capacity 298.15 K, C_p = 236.3 J·mol^{-1}·K^{-1}
Temperature range 124 to 293 K.
Data given graphically.
$C_p = 172.3 - 1.16T + 7.86\times10^{-3}T^2 - 1.09\times10^{-5}T^3$ J·mol^{-1}·K^{-1} (124 to 150 K; 240 to 293 K).
C_p value calculated from equation.
Phase Changes
c,II/c,I 150–240 K, ΔH = 702 J·mol^{-1}
ΔS = 3.55 J·mol^{-1}·K^{-1}
Molecular Weight 205.0515
Wiswesser Line Notation T5NØJ Ø-MN-- CO 3
Evaluation C (C_p), A (Phase changes)

$C_7H_4MnNO_3$ (c) 83CHH/POM
Azacymantrene; Pyrroyl manganese tricarbonyl
Heat Capacity 298.15 K, C_p = 216.2 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 250.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 305 K, ΔH = 1910 J·mol^{-1}
ΔS = 6.3 J·mol^{-1}·K^{-1}
c,I/liq 315.5 K, ΔH = 13010 J·mol^{-1}
ΔS = 41 J·mol^{-1}·K^{-1}
Molecular Weight 205.0515
Wiswesser Line Notation T5NØJ Ø-MN-- CO 3
Evaluation A

$C_7H_5BrO_2$ (c) 87FER/PIL
2-Bromobenzoic acid
Heat Capacity 298.15 K, C_p = 153.8 J·mol^{-1}·K^{-1}
One temperature.
Value given as C_p = 0.765 J·K^{-1}·g^{-1}.
Molecular Weight 201.0193
Wiswesser Line Notation QVR BE
Evaluation C

$C_7H_5BrO_2$ (c) 87FER/PIL
3-Bromobenzoic acid
Heat Capacity 298.15 K, C_p = 151.4 J·mol^{-1}·K^{-1}
One temperature.
Value given as C_p = 0.753 J·K^{-1}·g^{-1}.
Molecular Weight 201.0193
Wiswesser Line Notation QVR CE
Evaluation C

$C_7H_5BrO_2$ (c) 87FER/PIL
4-Bromobenzoic acid
Heat Capacity 298.15 K, C_p = 151.4 J·mol^{-1}·K^{-1}
One temperature.
Value given as C_p = 0.753 J·K^{-1}·g^{-1}.
Molecular Weight 201.0193
Wiswesser Line Notation QVR DE
Evaluation B

$C_7H_5Cl_3$ (liq) 87GOA/BOE
Benzotrichloride; α,α,α-Trichlorotoluene
Phase Changes
c,I/liq 235.99 K, ΔH = 13950 J·mol^{-1}
ΔS = 59.11 J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation GXGGR
Evaluation A

$C_7H_5F_3O_2$ (liq) 62GOO/LAC
3-Trifluoromethylbenzoic acid; *m*-Trifluorotoluic acid
Heat Capacity 298.15 K, C_p = 223.6 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 178.1105
Wiswesser Line Notation QV1R CXGGG
Evaluation B

C_7H_5N (liq) 83BYK/LEB
Benzonitrile
Heat Capacity 298.15 K, C_p = 165.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 209.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 260.33 K, ΔH = 10980 J·mol^{-1}
ΔS = 42.16 J·mol^{-1}·K^{-1}
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 84BYK/KIP
Benzonitrile
Heat Capacity 298.15 K, C_p = 165.2 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Phase Changes
c,I/liq 260.33 K, ΔH = 10980 J·mol^{-1}
ΔS = 42.16 J·mol^{-1}·K^{-1}
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 84LEB/BYK2
Benzonitrile
Heat Capacity 298.15 K, C_p = 165.2 J·mol^{-1}·K^{-1}
Temperature range 25 to 330 K.
Entropy 298.15 K, S = 209.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 260.332 K, ΔH = 10980 J·mol^{-1}
ΔS = 42.16 J·mol^{-1}·K^{-1}
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

C_7H_5N (liq) 85LEB/BYK
Benzonitrile
Heat Capacity 298.15 K, C_p = 165.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 209.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 260.33 K, ΔH = 10980 J·mol^{-1}
ΔS = 42.16 J·mol^{-1}·K^{-1}
Molecular Weight 103.1232
Wiswesser Line Notation NCR
Evaluation A

$C_7H_6NO_2$ (c) 72BOO/HAU
4-Nitrobenzoic acid
Phase Changes
c/liq 512.35 K, ΔH = 36900 J·mol^{-1}
ΔS = 72.0 J·mol^{-1}·K^{-1}
Molecular Weight 167.1208
Wiswesser Line Notation WNR DVQ
Evaluation C

$C_7H_6N_2$ (c) 87JIM/ROU
Benzimidazole
Heat Capacity 298.15 K, C_p = 128.8 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.09 J·K^{-1}·g^{-1}.
Molecular Weight 118.1378
Wiswesser Line Notation T56 BM DNJ
Evaluation B

$C_7H_6N_2$ (c) 87JIM/ROU
Indazole
Heat Capacity 298.15 K, C_p = 128.8 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.09 J·K^{-1}·g^{-1}.
Molecular Weight 118.1378
Wiswesser Line Notation T56 BMNJ
Evaluation B

$C_7H_6O_2$ (c) 57DAV/STA
Benzoic acid
Heat Capacity 298.15 K, C_p = 147.02 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 167.82 J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation B

$C_7H_6O_2$ (c) 75TAT/MAT
Benzoic acid
Heat Capacity 299.62 K, C_p = 147.07 J·mol^{-1}·K^{-1}
Temperature range 12 to 304 K
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 80SHA/LYU
Benzoic acid
Heat Capacity 298.15 K, C_p = 146.65 J·mol^{-1}·K^{-1}
Temperature range 20 to 300 K.
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_2$ (c) 88TOR/BAR
Benzoic acid
Phase Changes
liq/g 335 K, $\Delta H = 87450$ J·mol^{-1}
$\Delta S = 261.0$ J·mol^{-1}·K^{-1}
c/g 298.15 K, $\Delta H = 89230$ J·mol^{-1}.
$\Delta S = 299.3$ J·mol^{-1}·K^{-1}
Molecular Weight 122.1232
Wiswesser Line Notation QVR
Evaluation A

$C_7H_6O_3$ (c) 81LEB/RYA
3,4-Dihydroxybenzaldehyde
Heat Capacity $C_p = 205.7$ J·mol^{-1}·K^{-1}
Temperature range 298 to 413 K.
Data given over temperature range.
Heat capacity is an average value.
Molecular Weight 138.1226
Wiswesser Line Notation VHR CQ DQ
Evaluation B

C_7H_7F (liq) 62GOO/LAC
4-Fluorotoluene
Heat Capacity 298.15 K, $C_p = 172.3$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 110.1307
Wiswesser Line Notation FR D1
Evaluation B

$C_7H_7NO_3$ (c) 81LEB/RYA
p-Nitroanisole; 4-Nitromethoxybenzene
Heat Capacity $C_p = 279.9$ J·mol^{-1}·K^{-1}
Temperature range 298 to 320 K.
Data given over temperature range.
Molecular Weight 153.1372
Wiswesser Line Notation WNR DO1
Evaluation B

C_7H_7NS (c) 82SAB/TOR
Thiobenzamide
Heat Capacity 298 K, $C_p = 152.8$ J·mol^{-1}·K^{-1}
One temperature.
C_p given as 1.114 J·K^{-1}·g^{-1}.
Phase Changes
c/g 298.15 K, $\Delta H = 97200$ J·mol^{-1}
$\Delta S = 326.0$ J·mol^{-1}·K^{-1}
Molecular Weight 137.1990
Wiswesser Line Notation ZYR&US
Evaluation B

C_7H_8 (liq) 74RAJ/SUB
Toluene
Heat Capacity 298.15 K, $C_p = 156.8$ J·mol^{-1}·K^{-1}
Temperature range 298.15 to 323.15 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 75HOL/ZIE
Toluene
Heat Capacity 298.15 K, $C_p = 156.99$ J·mol^{-1}·K^{-1}
Temperature range 165 to 312 K.
$C_p = 187.43814 - 0.73026493T + 0.0029613602T^2 - 2.8661704\times10^{-6}T^3$ J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 178.166 K
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 76FOR/BEN2
Toluene
Heat Capacity 298.15 K, $C_p = 157.026$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A
Data from 76FOR/BEN.

C_7H_8 (liq) 84STE/OLS
Toluene
Heat Capacity 298.15 K, $C_p = 158.7$ J·mol^{-1}·K^{-1}
Temperature range 266 to 318 K.
C_p given as 0.4117 cal·g^{-1}·C^{-1}.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 86RED
Toluene
Heat Capacity 303.15 K, $C_p = 159.9$ J·mol^{-1}·K^{-1}
Temperature range 303.15, 313.15 K.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 86TAR/AIC
Toluene
Heat Capacity 298.15 K, $C_p = 158.70$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation B

C_7H_8 (liq) 88SHI/OGA
Toluene
Heat Capacity 298.15 K, $C_p = 155.96$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation 1R
Evaluation A

C_7H_8 (liq) 78STE
Quadricyclane;
Tetracyclo[3.2.0.0.^{2,7}0^{4,6}]heptane
Heat Capacity 298.15 K, $C_p = 157.6$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation L435 B3 2AB GTJ
Evaluation B

C_7H_8 (liq) 78STE
Norbornadiene; Bicyclo[2.2.1]hept-2,5-diene
Heat Capacity 298.15 K, $C_p = 161.2$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 92.1402
Wiswesser Line Notation L55 A CU FUTJ
Evaluation B

$C_7H_8N_2O$ (c) 87FER/DEL
Phenylurea; Monophenylurea
Phase Changes
c/liq 420.6 K, $\Delta H = 23680$ J·mol^{-1}
$\Delta S = 56.3$ J·mol^{-1}·K^{-1}
Molecular Weight 136.1530
Wiswesser Line Notation ZVMR
Evaluation A

C_7H_8O (liq) 1889EYK
Anisole; Methyl phenyl ether; Methoxybenzene
Phase Changes
c/liq 293.2 K, $\Delta H = 17029$ J·mol^{-1}
$\Delta S = 58.1$ J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation C

C_7H_8O (liq) 75FEN/HAR
Anisole; Methyl phenyl ether; Methoxybenzene
Heat Capacity 298.15 K, $C_p = 199.0$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation B

C_7H_8O (liq) 87GOA/BOE
Anisole; Methyl phenyl ether; Methoxybenzene
Phase Changes
c,I/liq 268.73 K, $\Delta H = 12890$ J·mol^{-1}
$\Delta S = 48.0$ J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation 1OR
Evaluation A

C_7H_8O (c) 82POE/FAN
2-Methylphenol; *o*-Hydroxytoluene; *o*-Cresol
Phase Changes
c/liq 303.0 K, $\Delta H = 13938$ J·mol^{-1}
$\Delta S = 46.00$ J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR B1
Evaluation A

C_7H_8O (liq) 82POE/FAN
3-Methylphenol; *m*-Hydroxytoluene; *m*-Cresol
Phase Changes
c/liq 285.0 K, $\Delta H = 9413$ J·mol^{-1}
$\Delta S = 33.03$ J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR C1
Evaluation A

C_7H_8O (c) 1889EYK
4-Methylphenol; *p*-Hydroxytoluene; *p*-Cresol
Phase Changes
c/liq 309 K, $\Delta H = 12247$ J·mol^{-1}
$\Delta S = 39.6$ J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation C

C_7H_8O (c) 82POE/FAN
4-Methylphenol; *p*-Hydroxytoluene; *p*-Cresol
Phase Changes
c/liq 309.0 K, $\Delta H = 11887$ J·mol^{-1}
$\Delta S = 38.47$ J·mol^{-1}·K^{-1}
Molecular Weight 108.1396
Wiswesser Line Notation QR D1
Evaluation A

C_7H_9N (liq) 87LES/LIC
N-Methylaniline
Heat Capacity 298 K, $C_p = 207.1$ J·mol^{-1}·K^{-1}
Temperature range 220 to 325 K.
Phase Changes
c/liq 216 K
Molecular Weight 107.1548
Wiswesser Line Notation 1MR
Evaluation B

C_7H_9N (liq) 86STE/CHI
2,3-Dimethylpyridine; 2,3-Lutidine
Heat Capacity 298.15 K, $C_p = 189.55$ J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 243.70$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 47.350 K
c,I/liq 258.565 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 C1
Evaluation A

C_7H_9N (liq) 86STE/CHI
2,4-Dimethylpyridine
Heat Capacity 298.15 K, $C_p = 184.76$ J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 248.50$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 209.415 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 D1
Evaluation A

C_7H_9N (liq) 86STE/CHI
2,5-Dimethylpyridine
Heat Capacity 298.15 K, $C_p = 184.70$ J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 248.81$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 182.200 K
c/liq 259.070 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 E1
Evaluation A

C_7H_9N (liq) 86STE/CHI
2,6-Dimethylpyridine
Heat Capacity 298.15 K, $C_p = 185.17$ J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, $S = 244.24$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 35.816 K
c,I/liq 267.033 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ B1 F1
Evaluation A

C_7H_9N (liq) 84POD/RAC
3,4-Dimethylpyridine
Heat Capacity 298 K, $C_p = 196$ J·mol^{-1}·K^{-1}
Temperature range 265 to 380 K.
Data graphically only.
Value given is estimated from graph.
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ C_1 D1
Evaluation B
Specific heat anomaly with peak at 293.5 K,
$\Delta H = 65.6$ J·mol^{-1},
$\Delta S = 0.16$ J·mol^{-1}·K^{-1}.
Temperature range of anomaly is 280 to 310 K.

C_7H_9N (liq) 86STE/CHI
3,4-Dimethylpyridine
Heat Capacity 298.15 K, C_p = 191.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 240.72 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 241.100 K
c,I/liq 262.704 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ C1 D1
Evaluation A

C_7H_9N (liq) 86STE/CHI
3,5-Dimethylpyridine
Heat Capacity 298.15 K, C_p = 184.55 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 241.72 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 266.823 K
Molecular Weight 107.1548
Wiswesser Line Notation T6NJ C1 E1
Evaluation A

C_7H_9N (c) 1889EYK
4-Methylaniline; *p*-Toluidine
Phase Changes
c/liq 315.6 K, ΔH = 17280 J·mol^{-1}
Molecular Weight 107.1548
Wiswesser Line Notation ZR D1
Evaluation C

$C_7H_8O_2 \cdot H_2O$ (c) 82VII/GAM
Orcinol monohydrate; 3,5-Dihydroxytoluene monohydrate
Phase Changes
c/liq 328.0 K, ΔH = 26360 J·mol^{-1}
ΔS = 80.4 J·mol^{-1}·K^{-1}
Molecular Weight 142.1542
Wiswesser Line Notation QR CQ E1 &QH
Evaluation B

C_7H_9NO (c) 81LEB/RYA
p-Anisidine
Heat Capacity C_p = 236.0 J·mol^{-1}·K^{-1}
Temperature range 298 to 320 K.
Data given over temperature range.
Molecular Weight 123.1542
Wiswesser Line Notation ZR DO1
Evaluation B

$C_6H_7N \cdot CH_2O$ (c) 82KIS/SAN
Aniline-formaldehyde
Heat Capacity C_p = 132.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 303 K.
C_p data given as 1.0736 J·K^{-1}·g^{-1} over a 25 to 30 °C temperature range.
Molecular Weight 123.1542
Wiswesser Line Notation ZR &VH
Evaluation C
C_p data given for 1:1 molar proportion of aniline formaldehyde.
C_p data also given for the solid compounds of molar proportion: 1:2, 1:3, 1:4, 1:4.5, 1:4.75, 1:5, 1:7, 2:1 and 4:1.

C_7H_{10} (c) 78STE
Nortricyclene; Tricyclo[2.2.1.0^{2,6}]heptane
Heat Capacity 298.15 K, C_p = 129.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1560
Wiswesser Line Notation L535 B 1A GTJ
Evaluation B

C_7H_{10} (liq) 78STE
Norbornene; Bicyclo[2.2.1]heptene
Heat Capacity 298.15 K, C_p = 129.9 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 94.1560
Wiswesser Line Notation L55 A CUTJ
Evaluation B

$C_7H_{10}N_2O$ (c) 80BYS
6,7-Diazatricyclo[3.2.2.0^{2,4}]non-6-ene N-oxide
Phase Changes
c,II/c,I 372.6 K, ΔH = 15800 J·mol^{-1}
ΔS = 42.4 J·mol^{-1}·K^{-1}
c,I/liq 411.4 K, ΔH = 2600 J·mol^{-1}
ΔS = 6.32 J·mol^{-1}·K^{-1}
Molecular Weight 138.1692
Wiswesser Line Notation T366/DI 2AC I ENUNTJ EUO
Evaluation A

$C_7H_{10}N_2O_2$ (c) 84ZIE/ZIE
1,3,6-Trimethyluracil
Phase Changes
c/liq 384.5 K, ΔH = 21200 J·mol^{-1}
ΔS = 55.1 J·mol^{-1}·K^{-1}
Molecular Weight 154.1682
Wiswesser Line Notation T6NVNVJ A1 C1 F1
Evaluation B

C_7H_{12} (c) 78STE
Norbornane; Bicyclo[2.2.1]heptane
Heat Capacity 298.15 K, C_p = 151.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 96.1718
Wiswesser Line Notation L55 ATJ
Evaluation B

C_7H_{12} (liq) 88LEB/KUL
4-Methylcyclohexene
Heat Capacity 298.15 K, C_p = 180.42 J·mol^{-1}·K^{-1}
Temperature range 13.4 to 350 K.
Entropy 298.15 K, S = 253.01 J·mol^{-1}·K^{-1}
Molecular Weight 96.1718
Wiswesser Line Notation L6UTJ D1
Evaluation A

C_7H_{12} (liq) 89LEB/SMI

cis-Cycloheptene

Heat Capacity 298.15 K, C_p = 171.7 J·mol^{-1}·K^{-1}

Temperature range 0 to 310 K.

Entropy 298.15 K, S = 241.0 J·mol^{-1}·K^{-1}

Phase Changes

c,III/c,II 154.22 K, ΔH = 7070 J·mol^{-1}; ΔS = 45.8 J·mol^{-1}·K^{-1}

c,II/c,I 208.26 K ΔH = 730 J·mol^{-1}; ΔS = 3.5 J·mol^{-1}·K^{-1}

c,I/liq 217.75 K ΔH = 820 J·mol^{-1}; ΔS = 4.1 J·mol^{-1}·K^{-1}

Molecular Weight 96.1718

Wiswesser Line Notation L7UTJ -C

Evaluation A

T_1(glass) = 97 K; T_2(glass) = 135 K

$(C_7H_{12})_n$ (liq) 80LEB/MUK

Butadiene-propylene copolymer

Heat Capacity 298.15 K, C_p = 192.4 J·mol^{-1}·K^{-1}

Temperature range 8 to 330 K.

Entropy 298.15 K, S = 209.0 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 262 K, ΔH = 7800 J·mol^{-1}; ΔS = 29.8 J·mol^{-1}·K^{-1}

100% crystallinity.

Molecular Weight 96.1718

Wiswesser Line Notation /*1Y1&2U2*/

Evaluation A

T(glass) = 198 K.

$C_7H_{12}O_2$ (liq) 85KAR/ABD2

Butyl acrylate

Phase Changes

c/liq 209.5 K, ΔH = 17307 J·mol^{-1}; ΔS = 82.61 J·mol^{-1}·K^{-1}

Molecular Weight 128.1706

Wiswesser Line Notation 4OV1U1

Evaluation A

$C_7H_{13}LiO_2$ (c) 86FRA/NGE

Lithium heptanoate

Heat Capacity 300 K, C_p = 231.72 J·mol^{-1}·K^{-1}

Temperature range 5 to 350 K.

Entropy 300 K, S = 231.06 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 317.08 K, ΔH = 5840 J·mol^{-1}; ΔS = 18.52 J·mol^{-1}·K^{-1}

Molecular Weight 136.1195

Wiswesser Line Notation OV6 .LI

Evaluation A

$C_7H_{13}NO$ (c) 62KOL/PAU

ζ-Enantholactam

Heat Capacity 295.00 K, C_p = 205.1 J·mol^{-1}·K^{-1}

Temperature range 60 to 350 K.

Entropy 298.15 K, S = 190.1 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 310.295 K, ΔH = 13775 J·mol^{-1}; ΔS = 44.4 J·mol^{-1}·K^{-1}

Molecular Weight 127.1835

Wiswesser Line Notation T8MVTJ

Evaluation B

$C_7H_{13}O_2Tl$ (c) 76MEI/SEY

Thallium heptanoate

Phase Changes

c,II/c,I 299 K, ΔH = 2761 J·mol^{-1}; ΔS = 9.20 J·mol^{-1}·K^{-1}

c,I/liq 419 K, ΔH = 6276 J·mol^{-1}; ΔS = 15.1 J·mol^{-1}·K^{-1}

Solid-mesophase.

liq/liq 501 K, ΔH = 3138 J·mol^{-1}; ΔS = 6.28 J·mol^{-1}·K^{-1}

Mesophase-isotropic.

Molecular Weight 333.5485

Wiswesser Line Notation OV6 .TL

Evaluation B

$C_7H_{13}O_2Tl$ (c) 84FER/LOP

Thallium heptanoate

Heat Capacity 320 K, C_p = 318 J·mol^{-1}·K^{-1}

Temperature range 320 to 480 K.

Phase Changes

c,II/c,I 301.9 K, ΔH = 2652 J·mol^{-1}; ΔS = 8.81 J·mol^{-1}·K^{-1}

c,I/liq 420.7 K, ΔH = 6302 J·mol^{-1}; ΔS = 15.0 J·mol^{-1}·K^{-1}

Solid-mesophase.

Molecular Weight 333.5485

Wiswesser Line Notation OV6 .TL

Evaluation A

Mesophase to isotropic liquid phase change data also given:

502.0 K; ΔH = 3301 J·mol^{-1}; ΔS = 6.57 J·mol^{-1}·K^{-1}.

$C_7H_{13}O_2Tl$ (c) 85NGE/LOP

Thallium heptanoate

Heat Capacity 298.15 K, C_p = 367.50 J·mol^{-1}·K^{-1}

Temperature range 5 to 500 K. Estimated value.

Entropy 298.15 K, S = 320.77 J·mol^{-1}·K^{-1}

Phase Changes

c,VI/c,V 262.8 K, ΔH = 1966 J·mol^{-1}; ΔS = 7.44 J·mol^{-1}·K^{-1}

c,V/c,IV 267.8 K, ΔH = 1167 J·mol^{-1}; ΔS = 4.36 J·mol^{-1}·K^{-1}

c,IV/c,III 271.7 K, ΔH = 1176 J·mol^{-1}; ΔS = 4.32 J·mol^{-1}·K^{-1}

c,III/c,II 296.2 K, ΔH = 2956 J·mol^{-1}; ΔS = 10.02 J·mol^{-1}·K^{-1}

c,II/c,I 300.9 K, ΔH = 2546 J·mol^{-1}; ΔS = 8.40 J·mol^{-1}·K^{-1}

c,I/liq 420.7 K

Solid-mesomorphic liquid.

Molecular Weight 333.5485

Wiswesser Line Notation OV6 .TL

Evaluation A

Mesomorphic liquid-isotropic liquid transition at 502.7 K.

$C_7H_{13}O_2Tl$ (c) 89LAB/LOP
Thallium heptanoate
Heat Capacity 298.15 K, C_p = 354.19 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 330.83 J·mol^{-1}·K^{-1}
Phase Changes

c,IV'/c,III'	269.3 K,	ΔH = 1413 J·mol^{-1}
		ΔS = 5.24 J·mol^{-1}·K^{-1}
c,III'/c,II	271.8 K,	ΔH = 1413 J·mol^{-1}
		ΔS = 5.15 J·mol^{-1}·K^{-1}
c,V/c,IV	262.3 K,	ΔH = 2087 J·mol^{-1}
		ΔS = 7.98 J·mol^{-1}·K^{-1}
c,IV/c,III	267.9 K,	ΔH = 1214 J·mol^{-1}
		ΔS = 4.49 J·mol^{-1}·K^{-1}
c,III/c,II	272.4 K,	ΔH = 1588 J·mol^{-1}
		ΔS = 5.82 J·mol^{-1}·K^{-1}
c,II/c,I	300.96 K,	ΔH = 3009 J·mol^{-1}
		ΔS = 9.18 J·mol^{-1}·K^{-1}
c,I/liq	420.7 K,	ΔH = 6302 J·mol^{-1}
		ΔS = 15.0 J·mol^{-1}·K^{-1}
c,I/mesophase.		
c/liq	502.0 K,	ΔH = 3301 J·mol^{-1}
		ΔS = 6.57 J·mol^{-1}·K^{-1}

Mesophase/isotropic liquid.
Molecular Weight 333.5485
Wiswesser Line Notation OV6 .TL
Evaluation A

C_7H_{14} (liq) 75HOL/ZIE
Methylcyclohexane
Heat Capacity 298.15 K, C_p = 184.84 J·mol^{-1}·K^{-1}
Temperature range 144 to 312 K.
C_p = 129.88277 − 0.0054107773T + 7.9975642×10$^{-4}T^2$ J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 146.550 K
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

C_7H_{14} (liq) 88SHI/OGA2
Methylcyclohexane
Heat Capacity 298.15 K, C_p = 184.38 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 98.1876
Wiswesser Line Notation L6TJ A1
Evaluation A

$C_7H_{14}O$ (liq) 87MIL/FEN2
3-Methylhexanal
Heat Capacity 323.15 K, C_p = 245.94 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 114.1870
Wiswesser Line Notation VH1Y3
Evaluation A

$C_7H_{14}O$ (liq) 87MIL/FEN2
3,4-Dimethylpentanal
Heat Capacity 323.15 K, C_p = 235.60 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 114.1870
Wiswesser Line Notation VH1YY
Evaluation A

$C_7H_{14}O$ (liq) 82DYA/VAS
Heptanal; Oenanthal; Enanthal; n-Heptaldehyde
Heat Capacity 298.15 K, C_p = 230.78 J·mol^{-1}·K^{-1}
Calculated from general equation:
C_p(J·mol^{-1}·K^{-1}) = (112.4±4.2) − (59.94±3.46)×10^{-2}T(K) + (10.93±0.74)×10$^{-4}T^2$ + (20.66±0.57)×n$_c$ (number of carbon atoms) + (2.65±0.19)×10^{-2}Tn$_c$.
Entropy 298.15 S = 335.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq ΔH = 22890 J·mol^{-1}
Molecular Weight 114.1870
Wiswesser Line Notation VH6
Evaluation B

$C_7H_{14}O$ (liq) 84VAS/PET
Heptanal; Oenanthal; Enanthal; n-Heptaldehyde
Heat Capacity 298.15 K, C_p = 230.15 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S = 335.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 229.20 K
Molecular Weight 114.1870
Wiswesser Line Notation VH6
Evaluation A

$C_7H_{14}O_2$ (liq) 86NIL/WAD
Ethyl-2,2-dimethylpropanoate
Heat Capacity 298.15 K, C_p = 251.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.1864
Wiswesser Line Notation 2OVX1&1&1
Evaluation A

$C_7H_{14}O_3$ (liq) 82BIR/SIK
2-Hydroxyethyl-2',2'-dimethylpropionate; 2-Hydroxyethyl pivalate
Heat Capacity 298.15 K, C_p = 308.0 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K. Equation only.
C_p = 15.79 + 1.337T − 0.001197T^2 J·mol^{-1}·K^{-1}.
Molecular Weight 146.1858
Wiswesser Line Notation Q2OVX1&1&1
Evaluation C

C_7H_{16} (liq) 76FIN/MES
3,3-Dimethylpentane
Heat Capacity 298.15 K, C_p = 214.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 305.6 J·mol^{-1}·K^{-1}
Phase Changes

c,II/c,I	132.7 K,	ΔH = 793.7 J·mol^{-1}
		ΔS = 5.98 J·mol^{-1}·K^{-1}
c,II/liq	138.20 K,	ΔH = 7642.5 J·mol^{-1}
		ΔS = 55.30 J·mol^{-1}·K^{-1}
c,I/liq	138.75 K,	ΔH = 6846.3 J·mol^{-1}
		ΔS = 49.34 J·mol^{-1}·K^{-1}

Molecular Weight 100.2034
Wiswesser Line Notation 2X2&1&1
Evaluation A

C_7H_{16} (liq) 76FIN/MES
2,3-Dimethylpentane
Heat Capacity 298.15 K, C_p = 218.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 297.1 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 2Y1&Y1&1
Evaluation A
T(glass) = 82.6 K.

C_7H_{16} (liq) 37VOL
n-Heptane
Heat Capacity 298 K, C_p = 223.0 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.532 cal/deg/gram.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 61MCC/MES
n-Heptane
Heat Capacity 298.15 K, C_p = 224.93 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
C_{sat}(liq) = 56.582 − 0.14490T + 5.7813×10$^{-4}T^2$ − 4.1667×10$^{-7}T^3$ cal·mol^{-1}·K^{-1}.
Phase Changes
c/liq 182.55 K, ΔH = 14037 J·mol^{-1}
ΔS = 76.89 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 75HOL/ZIE
n-Heptane
Heat Capacity 298.15 K, C_p = 224.19 J·mol^{-1}·K^{-1}
Temperature range 182 to 312 K.
C_p = 866.18820 − 9.9628490T + 0.054561085T^2 − 0.000130796340T^3 + 1.1957392×10$^{-7}T^4$ J·mol^{-1}·K^{-1}.
Phase Changes
c,I/liq 182.586 K
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 76FOR/BEN2
n-Heptane
Heat Capacity 298.15 K, C_p = 224.707 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 80KAL/JED
n-Heptane
Heat Capacity 297.860 K, C_p = 224.62 J·mol^{-1}·K^{-1}
Temperature range 185 to 300 K. Unsmoothed experimental datum.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 81GRO/ING
n-Heptane
Heat Capacity 298.15 K, C_p = 224.69 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 82ZAR
n-Heptane
Heat Capacity 298 K, C_p = 224.0 J·mol^{-1}·K^{-1}
Molecular Weight 100.2034
Temperature range 298, 323, 363 K.
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 83TAN/ZHO
n-Heptane
Heat Capacity 300 K, C_p = 225.33 J·mol^{-1}·K^{-1}
Temperature range 220 to 380 K.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

C_7H_{16} (liq) 84GRO/ING
n-Heptane
Heat Capacity 298.15 K, C_p = 224.71 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 84ROU/GRO
n-Heptane
Heat Capacity 298.15 K, C_p = 224.78 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation B

C_7H_{16} (liq) 88SHI/OGA
n-Heptane
Heat Capacity 298.15 K, C_p = 224.73 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 100.2034
Wiswesser Line Notation 7H
Evaluation A

$C_7H_{16}O$ (liq) 84ZEG/SOM
Heptanol; *n*-Heptyl alcohol
Heat Capacity 298.15 K, C_p = 273.67 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation C

$C_7H_{16}O$ (liq) 89VES/BAR
1-Heptanol
Heat Capacity 298.15 K C_p = 270.8 J·mol^{-1}·K^{-1}
Molecular Weight 116.2028
Wiswesser Line Notation Q7
Evaluation A

$C_7H_{17}NSi$ (liq) 75LEB/TSV
N-(β-Trimethylsilylethyl)ethylenimine
Heat Capacity 300 K, C_p = 300.8 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 300 K, S = 406.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 176.54 K, ΔH = 10623 J·mol^{-1}
ΔS = 60.2 J·mol^{-1}·K^{-1}
Molecular Weight 143.3035
Wiswesser Line Notation T3NTJ A2-SI-1&1&1
Evaluation A
T(glass) = 124.0 K.

$(C_7H_{17}NSi)_n$ (liq) 75LEB/TSV
Poly-N-(β-trimethylsilylethyl)ethylenimine
Heat Capacity 300 K, C_p = 287.4 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 300 K, S = 294.1 J·mol^{-1}·K^{-1}
Molecular Weight 143.3035
Wiswesser Line Notation /*2N*2-SI-1&1&1/
Evaluation A
T(glass) = 207.5 K.

$C_7H_{20}Si_2$ (c) 75GUS/KAR
Hexamethyldisilylmethane
Heat Capacity 298.15 K, C_p = 357.52 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Data given graphically.
Entropy 298.15 K, S = 515.89 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 140.70 K, ΔH = 11113 J·mol^{-1}
ΔS = 78.99 J·mol^{-1}·K^{-1}
liq/g 460.58 K, ΔH = 40250 J·mol^{-1}
ΔS = 98.99 J·mol^{-1}·K^{-1}
Molecular Weight 160.4060
Wiswesser Line Notation 1-SI-1&1&1-SI-1&1&1
Evaluation B

$C_7H_{20}Si_2$ (liq) 82GUS/KAR
Hexamethyldisilylmethane
Heat Capacity 298.15 K, C_p = 357.5 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S = 515.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 140.70 K, ΔH = 11113 J·mol^{-1}
ΔS = 78.99 J·mol^{-1}·K^{-1}
Molecular Weight 160.4060
Wiswesser Line Notation 1-SI-1&1&1-SI-1&1&1
Evaluation A

C_8D_8 (liq) 85LEB/LEB
Styrene-d_8
Heat Capacity 298.15 K, C_p = 201.9 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 243.74 K, ΔH = 10800 J·mol^{-1}
ΔS = 44.3 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation 1U1*R* &1/3/4/H-2 8
Evaluation B

$(C_8D_8)_n$ (gls) 83LEB/SMI
Polystyrene-d_8
Heat Capacity 298.15 K, C_p = 154.7 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S = 154.6 J·mol^{-1}·K^{-1}
Molecular Weight 112.2144
Wiswesser Line Notation /*YR&1*/ &1/2-BCDEF/4/H-2 8
Evaluation A

$(C_8H_3D_5)_n$ (gls) 83LEB/SMI
Polystyrene-d_5
Heat Capacity 298.15 K, C_p = 146.6 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S = 150.5 J·mol^{-1}·K^{-1}
Molecular Weight 109.1907
Wiswesser Line Notation /*YR&1*/ &2-BCDEF/H-2 5
Evaluation A

$C_8H_4Cl_2O_2$ (c) 79KAR/SAP
Terephthaloyl chloride
Heat Capacity 298.15 K, C_p = 207.9 J·mol^{-1}·K^{-1}
Temperature range 60 to 298 K.
Entropy 298.15 K, S = 226.1 J·mol^{-1}·K^{-1}
Molecular Weight 203.0244
Wiswesser Line Notation GVR DVG
Evaluation A

$C_8H_4N_2$ (c) 82KAR/SHV
1,2-Dicyanobenzene; *o*-Phthalonitrile
Heat Capacity 298.15 K, C_p = 161.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 480 K.
Entropy 298.15 K, S = 192.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 414.0 K, ΔH = 20000 J·mol^{-1}
ΔS = 48.26 J·mol^{-1}·K^{-1}
Molecular Weight 128.1330
Wiswesser Line Notation NCR BCN
Evaluation A

$C_8H_4N_2$ (c) 84RAB/KAR
1,2-Dicyanobenzene; *o*-Phthalonitrile
Heat Capacity 298.15 K, C_p = 161.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 500 K.
Entropy 298.15 K, S = 192.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 414.0 K, ΔH = 20000 J·mol^{-1}
ΔS = 48.26 J·mol^{-1}·K^{-1}
Molecular Weight 128.1330
Wiswesser Line Notation NCR BCN
Evaluation A

$C_8H_4N_2$ (c) 88LEB/BYK
1,4-Dicyanobenzene; Terephthalodinitrile
Heat Capacity 298.15 K, C_p = 161.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 183.0 J·mol^{-1}·K^{-1}
Molecular Weight 128.1330
Wiswesser Line Notation NCR DCN
Evaluation A

$C_8H_4O_3$ (c) 87BUS/MAS
Phthalic anhydride
Heat Capacity 298.15 K, C_p = 160.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 350 K.
Entropy 298.15 K, S = 180.0 J·mol^{-1}·K^{-1}
Molecular Weight 148.1178
Wiswesser Line Notation T56 BVOVJ
Evaluation A

C_8H_5Ag (c) 80BYK/KIP
Silver phenylacetylenide
Heat Capacity 298.15 K, C_p = 156.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 199.3 J·mol^{-1}·K^{-1}
Molecular Weight 208.9955
Wiswesser Line Notation -AG-1UU1R
Evaluation A

C_8H_5Cu (c) 79LEB/BYK
Copper phenylacetylenide
Heat Capacity 298.15 K, C_p = 154.0 J·mol^{-1}·K^{-1}
Temperature range 11 to 330 K.
Entropy 298.15 K, S = 173.8 J·mol^{-1}·K^{-1}
Molecular Weight 164.6735
Wiswesser Line Notation -CU-1UU1R
Evaluation A

C_8H_5Cu (c) 82BYK/LEB
Copper phenylacetylenide
Heat Capacity 298.15 K, C_p = 154.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 173.6 J·mol^{-1}·K^{-1}
Molecular Weight 164.6735
Wiswesser Line Notation -CU-1UU1R
Evaluation A

$(C_8H_5D_3)_n$ (gls) 83LEB/SMI
Polystyrene-d_3
Heat Capacity 298.15 K, C_p = 139.8 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S = 143.5 J·mol^{-1}·K^{-1}
Molecular Weight 107.1749
Wiswesser Line Notation /*YR&1*/ &3/6/H-2 3
Evaluation A

$C_8H_5MnO_3$ (c) 83CHH/POM
Cymantrene; Cyclopentadienyl manganese tricarboxyl
Heat Capacity 298.15 K, C_p = 214.79 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 259.35 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 75 to 135 K, ΔS = <1 J·mol^{-1}·K^{-1}
"Abnormally" high heat capacity.
c/liq 350 K, ΔH = 19300 J·mol^{-1}
ΔS = 55 J·mol^{-1}·K^{-1}
Molecular Weight 204.0637
Wiswesser Line Notation L5ØJ Ø-MN- -CO 3
Evaluation A

C_8H_6 (liq) 82LEB/BYK
Phenylacetylene
Heat Capacity 298.15 K, C_p = 180.10 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 480 K.
Entropy 298.15 K, S = 221.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 228.04 K, ΔH = 9460 J·mol^{-1}
ΔS = 41.5 J·mol^{-1}·K^{-1}
Molecular Weight 102.1354
Wiswesser Line Notation 1UU1R
Evaluation A

C_8H_6O (liq) 86CHI/NGU
2,3-Benzofuran
Heat Capacity 298.15 K, C_p = 178.70 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 215.59 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 232.000 K
c,I/liq 245.482 K
Molecular Weight 118.1348
Wiswesser Line Notation T56 BOJ
Evaluation A

$C_8H_7ClN_2O_2$ (c) 82CUE/SOL
2-Chloroisonitrosoacetanilide
Phase Changes
c/liq 429 K, ΔH = 29700 J·mol^{-1}
ΔS = 69.3 J·mol^{-1}·K^{-1}
Molecular Weight 198.6085
Wiswesser Line Notation QVU1VMR BG
Evaluation D

C_8H_7N (c) 81LEB/RYA
Indole; 1-Benzo[b]pyrrole
Heat Capacity C_p = 192.1 J·mol^{-1}·K^{-1}
Temperature range 298 to 318 K.
Data given over temperature range.
Molecular Weight 117.1500
Wiswesser Line Notation T56 BMJ
Evaluation B

C_8H_8 (liq) 43GUT/WES
Styrene
Entropy 298.15 K, S = 237.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 242.47 K, ΔH = 10950 J·mol^{-1}
ΔS = 45.16 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation A

C_8H_8 (liq) 85LEB/LEB
Styrene
Heat Capacity 298.15 K, C_p = 183.2 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 242.47 K, ΔH = 10950 J·mol^{-1}
ΔS = 45.2 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation 1U1R
Evaluation B

$(C_8H_8)_n$ (gls) 83LEB/SMI
Polystyrene
Heat Capacity 298.15 K, C_p = 127.5 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S = 134.8 J·mol^{-1}·K^{-1}
Molecular Weight 104.1512
Wiswesser Line Notation /*YR&1*/

$C_8H_8N_2O_2$ 82CUE/SOL
Isonitrosoacetanilide
Phase Changes
c/liq 448 K, ΔH = 10400 J·mol^{-1}
ΔS = 23.2 J·mol^{-1}·K^{-1}
Molecular Weight 164.1634
Wiswesser Line Notation QNU1VMR
Evaluation D

C_8H_8O (liq) 86CHI/NGU
4,5-Dihydro-2,3-benzofuran
Heat Capacity 298.15 K, C_p = 188.64 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 226.43 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 250.890 K
Molecular Weight 120.1506
Wiswesser Line Notation T56 BOT&J
Evaluation A

C_8H_9NO (c) 86NIL/WAD2
Acetanilide
Heat Capacity 298.15 K, C_p = 179.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 135.1652
Wiswesser Line Notation 1VMR
Evaluation B

$C_8H_9NO_3$ (c) 81LEB/RYA
p-Nitrophenetole; *p*-Nitroethoxybenzene
Heat Capacity C_p = 246.2 J·mol^{-1}·K^{-1}
Temperature range 298 to 328 K.
Data given over temperature range.
Molecular Weight 167.1640
Wiswesser Line Notation WNR DO2
Evaluation B

C_8H_{10} (liq) 86TAR/AIC
1,4-Dimethylbenzene; *p*-Xylene
Heat Capacity 298.15 K, C_p = 183.65 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation B

C_8H_{10} (liq) 88MES/FIN
1,4-Dimethylbenzene; *p*-Xylene
Heat Capacity 298.15 K, C_p = 182.219 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 247.154 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 286.405 K, ΔH = 17117.46 J·mol^{-1}
ΔS = 59.77 J·mol^{-1}·K^{-1}
Molecular Weight 106.1670
Wiswesser Line Notation 1R D1
Evaluation A

$C_8H_{10}N_4O_2$ (c) 80CES/STA
Caffeine
Heat Capacity 298 K, C_p = 173.2 J·mol^{-1}·K^{-1}
Temperature range 300 to 392 K.
Unsmoothed experimental data and equation given.
C_p = 41.4 + 0.104(T-298) cal·mol^{-1}·K^{-1}.
Data given at 298 *K* is an extrapolation by the author.
Phase Changes
c,II/c,I 426 K, ΔH = 940 J·mol^{-1}
ΔS = 2.2 J·mol^{-1}·K^{-1}
α to β form.
c,I/liq 512 K, ΔH = 5600 J·mol^{-1}
ΔS = 10.9 J·mol^{-1}·K^{-1}
β to liquid.
Molecular Weight 194.1926
Wiswesser Line Notation T56 BN DN FNVNVJ B1 F1 H1
Evaluation B
Data given for β form. β form is obtained by high temperature sublimation.

$C_8H_{10}O$ (liq) 75FEN/HAR
Ethyl phenyl ether
Heat Capacity 298.15 K, C_p = 228.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 122.1664
Wiswesser Line Notation 2OR
Evaluation B

$C_8H_{10}O$ (c) 82POE/FAN
2,3-Dimethylphenol
Phase Changes
c/liq 346.0 K, ΔH = 21024 J·mol^{-1}
ΔS = 60.76 J·mol^{-1}·K^{-1}
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 C1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
2,4-Dimethylphenol
Phase Changes
c/liq 299.0 K
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 D1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
2,5-Dimethylphenol
Phase Changes
c/liq 348.0 K, ΔH = 23376 J·mol^{-1}
ΔS = 67.17 J·mol^{-1}·K^{-1}
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 E1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
2,6-Dimethylphenol
Phase Changes
c/liq 318.9 K, ΔH = 18897 J·mol^{-1}
ΔS = 59.26 J·mol^{-1}·K^{-1}
Molecular Weight 122.1664
Wiswesser Line Notation QR B1 F1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
3,4-Dimethylphenol
Phase Changes
c/liq 334.0 K, ΔH = 18127 J·mol^{-1}
ΔS = 54.27 J·mol^{-1}·K^{-1}
Molecular Weight 122.1664
Wiswesser Line Notation QR C1 D1
Evaluation A

$C_8H_{10}O$ (c) 82POE/FAN
3,5-Dimethylphenol
Phase Changes
c/liq 336.8 K, ΔH = 17997 J·mol^{-1}
ΔS = 53.38 J·mol^{-1}·K^{-1}
Molecular Weight 122.1664
Wiswesser Line Notation QR C1 E1
Evaluation A

$C_8H_{10}O_3$ (c) 83GEI/NUR
cis-Cyclohexane-1,2-dicarboxylic anhydride
Heat Capacity 298.15 K, C_p = 207.4 J·mol^{-1}·K^{-1}
Temperature range 12 to 330 K.
Entropy 298.15 K, S = 202.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 304 K, ΔH = 5594 J·mol^{-1}
ΔS = 18.41 J·mol^{-1}·K^{-1}
Conformational transition.
c,II/c,I 310.5 K, ΔH = 845 J·mol^{-1}
ΔS = 2.72 J·mol^{-1}·K^{-1}
Conformational transition.
Molecular Weight 154.1652
Wiswesser Line Notation T56 BVOVTJ−C
Evaluation A

$C_8H_{11}N$ (liq) 86STE/CHI
2,6-Dimethylaniline
Heat Capacity 298.15 K, C_p = 238.86 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 251.35 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 284.598 K
Molecular Weight 121.1816
Wiswesser Line Notation ZR B1 F1
Evaluation A

C_8H_{12} (liq) 75LEB/LEB
Cycloocta-1,5-diene
Heat Capacity 298.15 K, C_p = 198.9 J·mol^{-1}·K^{-1}
Temperature range 6 to 320 K.
Entropy 298.15 K, S = 250.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 194.3 K, ΔH = -393 J·mol^{-1}
c,I/liq 203.983 K, ΔH = 9828 J·mol^{-1}
ΔS = 48.24 J·mol^{-1}·K^{-1}
Molecular Weight 108.1828
Wiswesser Line Notation L8 AU EUTJ
Evaluation A

$C_8H_{12}N_2O_2$ (liq) 83BYK/LEB2
1,6-Hexamethylene diisocyanate;
1,6-Diisocyanatohexane
Heat Capacity 298.15 K, C_p = 294.0 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Phase Changes
c/liq 206.06 K, ΔH = 18640 J·mol^{-1}
ΔS = 90.46 J·mol^{-1}·K^{-1}
Molecular Weight 136.1962
Wiswesser Line Notation OCN6NCO
Evaluation A

$C_8H_{12}N_2O_2$ (liq) 85LEB/BYK2
1,6-Hexamethylene diisocyanate;
1,6-Diisocyanatohexane
Heat Capacity 298.15 K, C_p = 294.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 420.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 206.064 K, ΔH = 18640 J·mol^{-1}
ΔS = 90.46 J·mol^{-1}·K^{-1}
Molecular Weight 168.1950
Wiswesser Line Notation OCN6NCO
Evaluation A

$(C_8H_{12}N_2O_2)_n$ (gls) 85LEB/BYK2
1,6-Hexamethylene diisocyanate polycyclotrimer
Heat Capacity 298.15 K, C_p = 222.7 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 242.0 J·mol^{-1}·K^{-1}
Molecular Weight 168.1950
Wiswesser Line Notation /T6NVNVNVJ A6NV&* C6NV&* E6NV&*/ 1/3
Evaluation A
T(glass) = 334 K.

$C_8H_{12}N_4$ (c) 81LEB/RYA
2,2'-Azodiisobutyrodinitrile;
Dinitrile-2,2'-azodiisobutyric acid
Heat Capacity 298.12 K, C_p = 238.1 J·mol^{-1}·K^{-1}
Temperature range 296 to 334 K.
Molecular Weight 164.2096
Wiswesser Line Notation NCX1&1&NUNX1&1&CN
Evaluation B

$C_8H_{12}N_4$ (c) 84LEB/GUT
2,2'-Azodiisobutyrodinitrile;
Dinitrile-2,2'-azodiisobutyric acid
Heat Capacity 298 K, C_p = 237.55 J·mol^{-1}·K^{-1}
Temperature range 296 to 335 K.
Phase Changes
c/liq 378 K
Molecular Weight 164.2096
Wiswesser Line Notation NCX1&1&NUNX1&1&CN
Evaluation B
ΔH sublimation = 76600 J·mol^{-1};
temperature range: 288 to 313 K.

C_8H_{14} (liq) 78LEB/LEB
Cyclooctene
Heat Capacity 298.15 K, C_p = 207.8 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 254.5 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 100 K
Glass transition.
c,II/c,I 190 K, ΔH = 635 J·mol^{-1}
ΔS = 3.34 J·mol^{-1}·K^{-1}
c,I/liq 259.15 K, ΔH = 1813 J·mol^{-1}
ΔS = 7.02 J·mol^{-1}·K^{-1}
Molecular Weight 110.1986
Wiswesser Line Notation L8UTJ
Evaluation A

$(C_8H_{14})_n$ (c) 78LEB/LEB
Polyoctenylene
Heat Capacity 298.15 K, C_p = 198.1 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 203.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 180 K, ΔH = 6336 J·mol^{-1}
ΔS = 35.2 J·mol^{-1}·K^{-1}
Glass transition.
c,I/liq 308 K, ΔH = 16760 J·mol^{-1}
ΔS = 54.4 J·mol^{-1}·K^{-1}
Molecular Weight 110.1986
Wiswesser Line Notation /L8TJ A* B*/
Evaluation A

$C_8H_{14}O$ (liq) 88BAG/GUR
6-Methyl-5-hepten-2-one
Heat Capacity 298.35 K, C_p = 268.8 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 126.1980
Wiswesser Line Notation 1YU3V1
Evaluation B

$C_8H_{14}O_2$ (liq) 85KAR/ABD
Butyl methacrylate
Heat Capacity 298.15 K, C_p = 273.7 J·mol^{-1}·K^{-1}
Temperature range 196 to 350 K.
C_p (J·kg^{-1}·K^{-1}) = 1344.3 + 1.9467 T.
C_p data calculated from equation.
Phase Changes
c/liq 196.8 K
Molecular Weight 142.1974
Wiswesser Line Notation 4OVY1&U1
Evaluation B

$C_8H_{14}O_2$ (liq) 85KAR/ABD2
Butyl methacrylate
Phase Changes
c/liq 196.8 K, ΔH = 13947 J·mol^{-1}
ΔS = 70.87 J·mol^{-1}·K^{-1}
Molecular Weight 142.1974
Wiswesser Line Notation 40VY1&U1
Evaluation A

$C_8H_{14}O_4$ (liq) 86NIL/WAD
Ethyleneglycol dipropanoate
Heat Capacity 298.15 K, C_p = 331.8 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 174.1962
Wiswesser Line Notation 2VO2OV2
Evaluation A

$C_8H_{15}NO_2$ (liq) 85KAR/ABD2
Dimethylaminoethyl methacrylate
Phase Changes
c/liq 237.7 K, $\Delta H = 16852$ J·mol^{-1}
$\Delta S = 70.90$ J·mol^{-1}·K^{-1}
Molecular Weight 157.2120
Wiswesser Line Notation 1UY1&VO2N1&1
Evaluation A

$C_8H_{15}O_2Tl$ (c) 76MEI/SEY
Thallium octanoate
Phase Changes
liq/liq 494 K, $\Delta H = 2720$ J·mol^{-1}
$\Delta S = 5.44$ J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,I/liq 403 K, $\Delta H = 4686$ J·mol^{-1}
$\Delta S = 11.7$ J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 347.5753
Wiswesser Line Notation OV7 .TL
Evaluation B

C_8H_{16} (liq) 88SHI/OGA2
Cyclooctane
Heat Capacity 298.15 K, $C_p = 215.78$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 112.2144
Wiswesser Line Notation L8TJ
Evaluation A

$C_8H_{16}O$ (liq) 80DYA/VAS
Octanal; Caprylaldehyde
Heat Capacity
Temperature range 50 to 350 K.
Phase Changes
c,I/liq 247.72 K, $\Delta H = 25860$ J·mol^{-1}
$\Delta S = 104.4$ J·mol^{-1}·K^{-1}
98.01 mol% purity.
Molecular Weight 128.2138
Wiswesser Line Notation VH7
Evaluation B
Manuscript deposited in Cent. Sci. Res. Inst. Tech. Eng. Petrochemicals, July 27, 1979.

$C_8H_{16}O$ (liq) 82DYA/VAS
Octanal; Caprylaldehyde
Entropy 298.15 K, $S = 365.4$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq $\Delta H = 26130$ J·mol^{-1}
Molecular Weight 128.2138
Wiswesser Line Notation VH7
Evaluation B

$C_8H_{16}O$ (liq) 84VAS/PET
Octanal; Caprylaldehyde
Heat Capacity 298.15 K, $C_p = 259.58$ J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 365.45$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 247.72 K
Molecular Weight 128.2138
Wiswesser Line Notation VH7
Evaluation A

$C_8H_{16}O_2$ (liq) 84GUS/SHU
Isoamyl propionate
Heat Capacity 298.15 K, $C_p = 285.2$ J·mol^{-1}·K^{-1}
Temperature range 205 to 348 K.
Unsmoothed experimental datum.
Interpolated to 298.15 K.
Molecular Weight 144.2132
Wiswesser Line Notation 2VO2Y
Evaluation C

$C_8H_{16}O_2$ (liq) 84VAS/PET
Butyl butanoate
Heat Capacity 300 K, $C_p = 281.9$ J·mol^{-1}·K^{-1}
Temperature range 180 to 370 K.
Phase Changes
c/liq 181.68 K, $\Delta H = 14930$ J·mol^{-1}
$\Delta S = 82.2$ J·mol^{-1}·K^{-1}
Molecular Weight 144.2132
Wiswesser Line Notation 4OV3
Evaluation A

$C_8H_{16}O_2$ (liq) 83GUS/KLI
Amyl propionate; Pentyl propionate
Heat Capacity 277.11 K, $C_p = 239.5$ J·mol^{-1}·K^{-1}
Temperature range 200 to 360 K.
Unsmoothed experimental datum.
C_p given as 1.661 J·g^{-1}·K^{-1}.
Molecular Weight 144.2132
Wiswesser Line Notation 50V2
Evaluation B

$C_8H_{16}O_2$ (liq) 84GUS/SHU
Amyl propionate; Pentyl propionate
Heat Capacity 298.15 K, $C_p = 245.2$ J·mol^{-1}·K^{-1}
Temperature range 205 to 348 K.
Unsmoothed experimental datum.
Interpolated to 298.15 K.
Molecular Weight 144.2132
Wiswesser Line Notation 5OV2
Evaluation C

$C_8H_{16}O_2$ (liq) 84VAS/PET
Hexyl ethanoate
Heat Capacity 300 K, $C_p = 282.8$ J·mol^{-1}·K^{-1}
Temperature range 210 to 370 K.
Phase Changes
c/liq 212.10 K, $\Delta H = 19830$ J·mol^{-1}
$\Delta S = 93.5$ J·mol^{-1}·K^{-1}
Molecular Weight 144.2132
Wiswesser Line Notation 6OV1
Evaluation A

$C_8H_{16}S$ (liq) 82TUT/GAB
1-Octanethiol; *n*-Octyl mercaptan
Heat Capacity 300 K, $C_p = 300.24$ J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 282.50 + 3.340\times10^{-2}T + 8.582\times10^{-5}T2$.
Molecular Weight 144.2744
Wiswesser Line Notation SH8
Evaluation B

$C_8H_{17}NO_2$ (c) 83SKO/SAB
8-Aminooctanoic acid
Heat Capacity 298 K, C_p = 251.7 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 159.2278
Wiswesser Line Notation Z7VQ
Evaluation B

C_8H_{18} (liq) 50AUE/SAG
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 300 K, C_p = 233.7 J·mol^{-1}·K^{-1}
Temperature range 300 to 366 K.
C_p given as 0.4980 Btu(lb)$^{-1}$(°R)$^{-1}$ at 80°F.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 74RAJ/SUB
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p = 237.8 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 323.15 K.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 76FOR/BEN2
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p = 238.871 J·mol^{-1}·K^{-1}
Average of three values.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 88COS/HUU
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p = 242.49 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation B

C_8H_{18} (liq) 88PER/AIC
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p = 242.49 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 88SHI/OGA
Isooctane; 2,2,4-Trimethylpentane
Heat Capacity 298.15 K, C_p = 239.71 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 1Y1&1X1&1&1
Evaluation A

C_8H_{18} (liq) 80SHA/LYU
n-Octane
Heat Capacity 298.15 K, C_p = 252.92 J·mol^{-1}·K^{-1}
Temperature range 65 to 300 K.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation A

C_8H_{18} (liq) 81GRO/ING
n-Octane
Heat Capacity 298.15 K, C_p = 254.07 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 82ZAR
n-Octane
Heat Capacity 298 K, C_p = 252.4 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 84ROU/GRO
n-Octane
Heat Capacity 298.15 K, C_p = 254.02 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 85LAI/GRO
n-Octane
Heat Capacity 298.15 K, C_p = 254.18 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 86TAR/AIC
n-Octane
Heat Capacity 298.15 K, C_p = 255.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation B

C_8H_{18} (liq) 88PER/AIC
n-Octane
Heat Capacity 298.15 K, C_p = 255.68 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 114.2302
Wiswesser Line Notation 8H
Evaluation A

$C_8H_{18}N_2$ (c) 80BYS
1,1-Dimethylazoethane
Phase Changes

c,II/c,I	242.6 *K*	ΔH = 4890 J·mol^{-1}
		ΔS = 20.2 J·mol^{-1}·K^{-1}
c,I//liq	258.6 *K*	ΔH = 10280 J·mol^{-1}
		ΔS = 39.7 J·mol^{-1}·K^{-1}

Molecular Weight 142.2443
Wiswesser Line Notation 1X1&1&NUNX1&1&1
Evaluation A

$C_8H_{18}N_2O$ (c) 80BYS
1,1-Dimethylazoxyethane
Phase Changes

c,II/c,I	268.0 *K*	ΔH = 8340 J·mol^{-1}
		ΔS = 31.1 J·mol^{-1}·K^{-1}
c,I//liq	288.4 *K*	ΔH = 11520 J·mol^{-1}
		ΔS = 39.9 J·mol^{-1}·K^{-1}

Molecular Weight 158.2437
Wiswesser Line Notation 1X1&1&NO&UNX1&1&1
Evaluation A

$C_8H_{18}N_2O_2$ (c) 84LEB/GUT
Bis-hydroxyethylpiperazine
Heat Capacity 298 K, C_p = 250.68 J·mol^{-1}·K^{-1}
Temperature range 293 to 311 K.
Phase Changes
c/liq 405 K, ΔH = 25900 J·mol^{-1}
ΔS = 64.0 J·mol^{-1}·K^{-1}
liq/g 551 K
Molecular Weight 174.2424
Wiswesser Line Notation T6N DNTJ A2Q D2Q
Evaluation B
ΔH sublimation = 104100 J·mol^{-1},
temperature range: 334 to 356 K.

$C_8H_{18}O$ (liq) 75FEN/HAR
Di-*tert*-butyl ether; 2,2,4,4-Tetramethyl-3-oxapentane
Heat Capacity 298.15 K, C_p = 276.1 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.2296
Wiswesser Line Notation 1X1&1&OX1&1&1
Evaluation B

$C_8H_{18}O$ (liq) 87COB/CAS
Di-*n*-butyl ether
Heat Capacity 298.15 K, C_p = 278.16 J·mol^{-1}·K^{-1}
One temperature.
Average of two measurements.
Molecular Weight 130.2296
Wiswesser Line Notation 4O4
Evaluation B

$C_8H_{18}O$ (liq) 87BUS/MAS
2-Ethylhexanol
Heat Capacity 298.15 K, C_p = 317.5 J·mol^{-1}·K^{-1}
Temperature range 13 to 350 K.
Entropy 298.15 K, S = 347.0 J·mol^{-1}·K^{-1}
Molecular Weight 130.2296
Wiswesser Line Notation Q1Y4&2
Evaluation A

$C_8H_{18}O$ (liq) 78RYB/EME
Isooctyl alcohol; 2-Methyl-1-heptanol
Heat Capacity 303.15 K, C_p = 327.8 J·mol^{-1}·K^{-1}
Temperature range 293.15 to 353.15 K.
C_p given as 2517 J·kg^{-1}·K^{-1}.
Molecular Weight 130.2296
Wiswesser Line Notation Q1Y5&1
Evaluation C

$C_8H_{18}O$ (liq) 84ZEG/SOM
1-Octanol; *n*-Octyl alcohol; Capryl alcohol
Heat Capacity 298.15 K, C_p = 305.55 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation C

$C_8H_{18}O$ (liq) 89VES/BAR
1-Octanol; *n*-Octyl alcohol; Capryl alcohol
Heat Capacity 298.15 K C_p = 304.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 130.2296
Wiswesser Line Notation Q8
Evaluation A

$C_8H_{18}O_3$ (liq) 87COB/CAS
2-(2-Butoxyethoxy)ethanol
Heat Capacity 298.15 K, C_p = 354.89 J·mol^{-1}·K^{-1}
One temperature.
Average of two measurements.
Molecular Weight 162.2284
Wiswesser Line Notation Q2O2O4
Evaluation B

$C_8H_{18}O_5$ (liq) 82ZAR
Tetraethylene glycol
Heat Capacity 298 K, C_p = 428.8 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 194.2272
Wiswesser Line Notation Q2O2O2O2Q
Evaluation B

$C_8H_{19}N$ (liq) 01KAH
Diisobutyl amine
Heat Capacity C_p = 129.2 J·mol^{-1}·K^{-1}
Temperature range 294.15 to 403.15 K.
Heat capacity is an average value over the temperature range.
Molecular Weight 129.2448
Wiswesser Line Notation 2YMY2
Evaluation D

$(C_8H_{19}NSi)_n$ (liq) 76LEB/EVS
Poly-N-(β-trimethylsilylethyl)azetidine
Heat Capacity 298 K, C_p = 318.0 J·mol^{-1}·K^{-1}
Temperature range 65 to 305 K.
Deposited in VINITI, No. 3786–75, 26 December 1975.
Entropy 298 K, S = 315.7 J·mol^{-1}·K^{-1}
Molecular Weight 157.3303
Wiswesser Line Notation /*3N*2-SI-1&1&1/
Evaluation B
T(glass) = 204.0 K.

$C_8H_{19}NSi$ (liq) 77LEB/RAB5
N-(β-Trimethylsilylethyl)trimethylenimine
Heat Capacity 298.15 K, C_p = 304.6 J·mol^{-1}·K^{-1}
Temperature range 7 to 305 K.
Entropy 298.15 K, S = 398.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 199.43 K, ΔH = 12900 J·mol^{-1}
ΔS = 64.6 J·mol^{-1}·K^{-1}
Molecular Weight 157.3303
Wiswesser Line Notation T4NTJ A2-SI-1&1&1
Evaluation A
T(glass) = 126.7 K.

$C_8H_{19}Cl_2NSiZn$ (liq) 76EVS/LEB
N-(β-Trimethylsilylethyl)azetidine, zinc chloride complex
Heat Capacity 298.15 K, C_p = 607.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Deposited in VINITI, No. 3824–75, 26 December 1975.
Entropy 298.15 K, S = 575.1 J·mol^{-1}·K^{-1}
Molecular Weight 312.7758
Wiswesser Line Notation T4NTJ A2-SI-1&1&1 &.ZN..G2
Evaluation B
Complex assumed 1:1.

$(C_8H_{19}Cl_2NSiZn)_n$ (liq) 76EVS/LEB
Poly-N-(β-Trimethylsilylethyl)azetidine, zinc chloride complex
Heat Capacity 298.15 K, C_p = 568.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Deposited in VINITI, No. 3824–75, 26 December 1975.
Entropy 298.15 K, S = 542.2 J·mol^{-1}·K^{-1}
Molecular Weight 312.7758
Wiswesser Line Notation /*3N*2-SI-1&1&1 &.ZN..G2/
Evaluation B
Complex assumed 1:1.

$C_8H_{20}Br_4FeN$ (c) 88NAV/PUE
Tetraethylammonium tetrabromo ferrate
Heat Capacity 298.15 K, C_p = 369.4 J·mol^{-1}·K^{-1}
Temperature range 50 to 300 K.
Entropy 298.15 K, S = 415.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 236.1 K, ΔH = 2428 J·mol^{-1}
ΔS = 10.2 J·mol^{-1}·K^{-1}
Molecular Weight 505.7157
Wiswesser Line Notation 2K2&2&2 .FE G4
Evaluation A

$C_8H_{20}Cl_4FeN$ (c) 88NAV/PUE
Tetraethylammonium tetrachloro ferrate
Heat Capacity 298.15 K, C_p = 374.8 J·mol^{-1}·K^{-1}
Temperature range 1.4 to 300 K.
Entropy 298.15 K, S = 490.2 J·mol^{-1}·K^{-1}
Phase Changes
c,V/c,IV 2.93 K
Neel point, lambda transition.
c,IV/c,IIII 234.7 K, ΔH = 2203 J·mol^{-1}
ΔS = 8.06 J·mol^{-1}·K^{-1}
First order transition.
c,III/c,II 217.5 K
c,II/c,I 226.6 K, ΔH = 2295 J·mol^{-1}
ΔS = 11.4 J·mol^{-1}·K^{-1}
First order transition.
Molecular Weight 327.9117
Wiswesser Line Notation 2K2&2&2 .FE G4
Evaluation A

$C_8H_{20}Ge$ (liq) 54STA/WAR
Tetraethylgermane
Phase Changes
c/liq 180.47 K, ΔH = 12406 J·mol^{-1}
ΔS = 68.74 J·mol^{-1}·K^{-1}
Molecular Weight 188.8360
Wiswesser Line Notation 2-GE-2&2&2
Evaluation B

$C_8H_{20}Ge$ (liq) 85RAB/SHE
Tetraethyl germane
Heat Capacity 298.15 K, C_p = 294.7 J·mol^{-1}·K^{-1}
Temperature range 8 to 300 K.
Entropy 298.15 K, S = 428.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 179.99 K, ΔH = 12312 J·mol^{-1}
ΔS = 68.00 J·mol^{-1}·K^{-1}
Molecular Weight 188.8360
Wiswesser Line Notation 2-GE-2&2&2
Evaluation A

$C_8H_{20}N_4$ (liq) 88BOB/KAM
N-[2-Aminoethyl)2-aminoethyl]piperazine
Heat Capacity 333 K, C_p = 391 J·mol^{-1}·K^{-1}
Temperature Range 333 to 473 K
Molecular Weight 172.2728
Wiswesser Line Notation T6M DNTJ D2M2Z
Evaluation D

$C_8H_{20}N_4$ (liq) 88BOB/KAM
N,N'-Di-(2-aminoethyl)piperazine
Heat Capacity 333 K, C_p = 407 J·mol^{-1}·K^{-1}
Temperature range 333 to 473 K
Molecular Weight 172.2728
Wiswesser Line Notation T6N DNTJ A2Z D2Z
Evaluation D

$C_8H_{20}Pb$ (liq) 54STA/WAR
Tetraethyl lead
Phase Changes
c/liq 142.94 K, ΔH = 8791 J·mol^{-1}
ΔS = 61.50 J·mol^{-1}·K^{-1}
Molecular Weight 323.4460
Wiswesser Line Notation 2-PB-2&2&2
Evaluation B

$C_8H_{20}Pb$ (liq) 89RAB/NIS2
Tetraethyllead
Heat Capacity 298.15 K, C_p = 307.4 J·mol^{-1}·K^{-1}
Temperature Range 5–315 K.
Entropy 298.15 K S = 464.6 J·mol^{-1}·K^{-1}
Phase Changes
c,III/liq 90.8 K
Glass/supercooled liquid transition
c,II/liq 141.4 K ΔH = 9110 J·mol^{-1}
ΔS = 64.43 J·mol^{-1}·K^{-1}
c,I/liq 139.41 K ΔH = 9091 J·mol^{-1}
ΔS = 65.21 J·mol^{-1}·K^{-1}
Molecular Weight 323.4460
Wiswesser Line Notation 2-PB-2&2&2
Evaluation A

$C_8H_{20}Si$ (liq) 54STA/WAR
Tetraethyl silicon
Phase Changes
c/liq 189.36 K, ΔH = 13012 J·mol^{-1}
ΔS = 68.70 J·mol^{-1}·K^{-1}
Molecular Weight 144.3315
Wiswesser Line Notation 2-SI-2&2&2
Evaluation B

$C_8H_{20}Sn$ (liq) 54STA/WAR
Tetraethyl tin
Phase Changes
c/liq 142.14 K, ΔH = 9146 J·mol^{-1}
ΔS = 64.35 J·mol^{-1}·K^{-1}
Molecular Weight 234.9360
Wiswesser Line Notation 2-SN-2&2&2
Evaluation B

$C_8H_{24}Ag_{13}I_{15}N_2$ (c) 85LIN/ARM
Bis-(tetramethylammonium iodide) tridecasilver iodide
Heat Capacity 282.93 K, C_p = 1076 J·mol^{-1}·K^{-1}
Temperature range 79 to 283 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 150 K, ΔS = 5.34 J·mol^{-1}·K^{-1}
Molecular Weight 3454.1425
Wiswesser Line Notation 1K1&1&1&1 2 .AG I 13
Evaluation A

$C_8H_{24}Cl_4FeN_2$ (c) 88RUI/LOP
Tetramethylammonium tetrachloroferrate
Heat Capacity 300 K, C_p = 424 J·mol^{-1}·K^{-1}
Temperature range 60 to 350 K.
Data given graphically.
C_p datum is graphical estimate.
Phase Changes
c,IV/c,III 240.0 K, ΔH = 859.6 J·mol^{-1}
ΔS = 3.68 J·mol^{-1}·K^{-1}
c,III/c,II 266.8 K, ΔH = 238.5 J·mol^{-1}
ΔS = 0.90 J·mol^{-1}·K^{-1}
c,II/c,I 281.0 K, ΔH = 2179.9 J·mol^{-1}
ΔS = 8.34 J·mol^{-1}·K^{-1}
Molecular Weight 345.9500
Wiswesser Line Notation 1K1&1&1 2 .FE G4
Evaluation B

$C_8H_{24}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(butylammonium) manganese II
Phase Changes
c,II/c,I 371 K, ΔH = 2.4 J·mol^{-1}
ΔS = 0.007 J·mol^{-1}·K^{-1}
Molecular Weight 345.0410
Wiswesser Line Notation 4ZH 2 .MN G4
Evaluation A

$C_8H_{24}Cl_4MnN_2$ (c) 88ZUB/LOP
Tetramethylammonium tetrachloromanganate
Heat Capacity 300 K, C_p = 424 J·mol^{-1}·K^{-1}
Temperature range 50 to 330 K.
Data given graphically and estimated from graph.
Phase Changes
c,V/c,IV 175.63 K, ΔH = 308 J·mol^{-1}
ΔS = 1.75 J·mol^{-1}·K^{-1}
c,IV/c,III 268.65 K, ΔH = 233 J·mol^{-1}
ΔS = 0.83 J·mol^{-1}·K^{-1}
c,III/c,II 292.3 K, ΔH = 5.8 J·mol^{-1}
ΔS = 0.02 J·mol^{-1}·K^{-1}
c,II/c,I 292.6 K, ΔH = 2079 J·mol^{-1}
ΔS = 7.98 J·mol^{-1}·K^{-1}
Molecular Weight 345.0410
Wiswesser Line Notation 1K1&1&1 2 .MN G4
Evaluation A

$C_8H_{23}N_5$ (liq) 88BOB/KAM
Tetraethylenepentamine
Heat Capacity 333 K, C_p = 460 J·mol^{-1}K^{-1}
Temperature Range 333 to 513 K.
Molecular Weight 189.3032
Wiswesser Line Notation Z2M2M2M2Z
Evaluation D

$C_8H_{24}Si_4O_4$ (liq) 81MEK/KAR
Octamethyltetrasiloxane
Heat Capacity 298.15 K, C_p = 509.6 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Data given graphically.
Entropy 298.15 K, S = 623.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 290.25 K, ΔH = 23765 J·mol^{-1}
ΔS = 81.80 J·mol^{-1}·K^{-1}
Molecular Weight 296.6172
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-
OTJ A1 A1 C1 C1 E1 E1 G1 G1
Evaluation A

$C_8H_{28}Ni_4Si$ (c) 81MEK/KAR
Octamethyltetrasilazane
Heat Capacity 298.15 K, C_p = 569.9 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Data given graphically.
Entropy 298.15 K, S = 599.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 367.67 K, ΔH = 25050 J·mol^{-1}
ΔS = 66.5 J·mol^{-1}·K^{-1}
Molecular Weight 387.1947
Wiswesser Line Notation T8-SI-M-SI-M-SI-M-SI-
MTJ A1 A1 C1 C1 E1 E1 G1 G1

$C_9H_6CrO_3$ (c) 78POM/CHH
Benzene chromium tricarbonyl
Heat Capacity 298.15 K, C_p = 151.3 J·mol^{-1}·K^{-1}
Temperature range 120 to 300 K.
Data given graphically.
$C_p = 38.17 + 2.37\times10^{-1}T + 3.77\times10^{-4}T^2 + 3.38\times10^{-7}T^3$ J·mol^{-1}·K^{-1} (120 to 300 K).
C_p value calculated from equation.
Molecular Weight 214.1406
Wiswesser Line Notation L6ØJ Ø-CR-- CO 3
Evaluation C (C_p), A (Phase changes)

C_9H_7Cu (c) 82BYK/LEB
Copper benzylacetylenide
Heat Capacity 298.15 K, C_p = 178.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 197.6 J·mol^{-1}·K^{-1}
Molecular Weight 178.7003
Wiswesser Line Notation -CU-1UU1R
Evaluation A

C_9H_7N (liq) 86STE/CHI
Quinoline
Heat Capacity 298.15 K, C_p = 194.90 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, S = 219.69 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 220.093 K
c,I/liq 238.369 K
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation A

C_9H_7N (liq) 88STE/ARC
Quinoline
Heat Capacity 298.15 K, C_p = 194.89 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 219.72 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 220.000 K, ΔH = 68.18 J·mol^{-1}
ΔS = 0.310 J·mol^{-1}·K^{-1}
c,I/liq 258.369 K, ΔH = 10662.90 J·mol^{-1}
ΔS = 41.27 J·mol^{-1}·K^{-1}
Molecular Weight 129.1610
Wiswesser Line Notation T66 BNJ
Evaluation A

C_9H_7N (liq) 88STE/ARC
Isoquinoline
Heat Capacity 298.15 K, C_p = 196.16 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K. Values calculated from graphically extrapolated heat capacity values.
Entropy 298.15 K, S = 215.98 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 221.000 K, ΔH = 0.00 J·mol^{-1}
c,II/c,I 275.000 K, ΔH = 0.00 J·mol^{-1}
c,I/liq 299.620 K, ΔH = 13544.17 J·mol^{-1}
ΔS = 45.20 J·mol^{-1}·K^{-1}
Molecular Weight 129.1610
Wiswesser Line Notation T66 CNJ
Evaluation A

C_9H_7N (c) 86STE/CHI
Isoquinoline
Heat Capacity 298.15 K, C_p = 177.68 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 171.06 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 219.600 K
c,II/c,I 275.000 K
c,I/liq 299.616 K
Molecular Weight 129.1610
Wiswesser Line Notation T66 CNJ
Evaluation A

C_9H_7NO (c) 81LEB/RYA
3-Indole aldehyde
Heat Capacity C_p = 220.5 J·mol^{-1}·K^{-1}
Temperature range 298 to 458 K.
Data given over temperature range.
Molecular Weight 145.1604
Wiswesser Line Notation T56 BMJ DVH
Evaluation B

C_9H_7O (liq) 86CHI/NGU
Chroman
Heat Capacity 298.15 K, C_p = 214.00 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 246.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.836 K
Molecular Weight 131.1537
Wiswesser Line Notation T66 BOJ

Evaluation A

C_9H_7O (liq) 86CHI/NGU
Isochroman
Heat Capacity 298.15 K, C_p = 217.81 J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, S = 247.04 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 277.503 K
Molecular Weight 131.1537
Wiswesser Line Notation T66 COJ
Evaluation A

$C_9H_8MnO_3P$ (c) 82POI/SOU
3,4-Dimethylphospholyl manganese tricarbonyl;
Dimethyl-3,4-phosphacymantrene
Phase Changes
c,II/c,I 275 K, ΔH = 190 J·mol^{-1}
ΔS = 0.69 J·mol^{-1}·K^{-1}
c,I/liq 300 K, ΔH = 19300 J·mol^{-1}
ΔS = 64 J·mol^{-1}·K^{-1}
Molecular Weight 250.0722
Wiswesser Line Notation T5PJ C1 D1 &–MN– CO 3
Evaluation A

$C_9H_8O_2$ (c) 86SIN/KUM
Cinnamic acid
Phase Changes
c/liq 406.15 K, ΔH = 22626 J·mol^{-1}
ΔS = 55.71 J·mol^{-1}·K^{-1}
Molecular Weight 148.1610
Wiswesser Line Notation QV1U1R
Evaluation A

$C_9H_8O_3$ (c) 83GEI/SAL
Endobicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid anhydride
Heat Capacity 298.15 K, C_p = 183.3 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298.15 K, S = 189.5 J·mol^{-1}·K^{-1}
Molecular Weight 164.1604
Wiswesser Line Notation T555/FJ 2AE J BVOV IUTJ
Evaluation A
There is an extended hump in the C_p curve between 50 and 150 K.

C_9H_9FeN (c) 84CHH/POM
Azaferrocene
Heat Capacity 298.15 K, C_p = 183.4 J·mol^{-1}·K^{-1}
Temperature range 70 to 290 K.
Entropy 298.15 K, S = 211.8 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,I′ 200 K, ΔH = 3000 J·mol^{-1}
ΔS = 15.0 J·mol^{-1}·K^{-1}
c,II/c,I′ 218 K, ΔH = −3800 J·mol^{-1}
ΔS = −17.4 J·mol^{-1}·K^{-1}
Molecular Weight 187.0238
Wiswesser Line Notation T5NØJ Ø-FE-- ØL5ØJ
Evaluation A
Metastable phase.

C_9H_9FeN (c) 84CHH/POM
Azaferrocene
Heat Capacity 298.15 K, C_p = 177.0 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 170.30 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 278.5 K, ΔH = 650 J·mol^{-1}
ΔS = 2.4 J·mol^{-1}·K^{-1}
c,II/c,I 289.5 K, ΔH = 6748 J·mol^{-1}
ΔS = 23.6 J·mol^{-1}·K^{-1}
Molecular Weight 187.0238
Wiswesser Line Notation T5NØJ Ø-FE-- ØL5ØJ
Evaluation A
Stable phase.

C_9H_9FeP (c) 84CHH/POM
Phosphaferrocene
Phase Changes
c,II/c,I 266 K, $\Delta H = 7330$ J·mol^{-1}
$\Delta S = 27.6$ J·mol^{-1}·K^{-1}
Molecular Weight 203.9909
Wiswesser Line Notation T5PØJ Ø-FE-- ØL5ØJ
Evaluation A
Stable phase.
A metastable phase transition is reported at $T = 210$ K.

C_9H_{10} (liq) 71LEB/RAB2
α-Methylstyrene
Heat Capacity 300 K, $C_p = 202.2$ J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, $S = 243.8$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 250.78 K, $\Delta H = 11924$ J·mol^{-1}
$\Delta S = 47.55$ J·mol^{-1}·K^{-1}
Molecular Weight 118.1780
Wiswesser Line Notation 1UY1&R
Evaluation B

$(C_9H_{10})_n$ (c) 71LEB/RAB2
Poly(α-methylstyrene)
Heat Capacity 300 K, $C_p = 149.2$ J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 300 K, $S = 134.7$ J·mol^{-1}·K^{-1}
Molecular Weight 118.1780
Wiswesser Line Notation /*1X*1&R/
Evaluation B

$C_9H_{10}N_2O_3$ (c) 82CUE/SOL
2-Methoxyisonitrosoacetanilide
Phase Changes
c/liq 422 K, $\Delta H = 27800$ J·mol^{-1}
$\Delta S = 65.9$ J·mol^{-1}·K^{-1}
Molecular Weight 194.1896
Wiswesser Line Notation QNU1VMR BO1
Evaluation D

$C_9H_{10}N_2O_3$ (c) 82CUE/SOL
4-Methoxyisonitrosoacetanilide
Phase Changes
c/liq 459 K, $\Delta H = 8300$ J·mol^{-1}
$\Delta S = 18.1$ J·mol^{-1}·K^{-1}
Molecular Weight 194.1896
Wiswesser Line Notation QNU1VMR DO1
Evaluation D

$C_9H_{10}O_2$ (c) 1889EYK
Phenylpropionic acid
Phase Changes
c/liq 321.6 K, $\Delta H = 15564$ J·mol^{-1}
$\Delta S = 48.4$ J·mol^{-1}·K^{-1}
Molecular Weight 150.1768
Wiswesser Line Notation QV2R
Evaluation C

$C_9H_{10}O_2$ (c) 87LES/LIC
Phenyl glycidyl ether
Heat Capacity 298 K, $C_p = 278.7$ J·mol^{-1}·K^{-1}
Temperature range 225 to 400 K.
Molecular Weight 150.1768
Wiswesser Line Notation T3OTJ B1OR
Evaluation B

$C_9H_{10}O_2$ (liq) 88LEB/BYK2
Phenyl glycidyl ether
Heat Capacity 298.15 K, $C_p = 276.0$ J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, $S = 274.9$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 276.79 K
Molecular Weight 150.1768
Wiswesser Line Notation T3OTJ B1OR
Evaluation A
Data also given for the vitreous state from 5 to 189 K, and for the supercooled liquid from 200 to 276.79 K.

$C_9H_{11}N$ (liq) 89STE/CHI2
1,2,3,4-Tetrahydroquinoline
Heat Capacity 298.15 K, $C_p = 236.04$ J·mol^{-1}·K^{-1}
Temperature range 10 to 440 K.
Entropy 298.15 K, $S = 240.36$ J·mol^{-1}·K^{-1}
Phase Changes
c,IV/c,III 61.7 K
c,III/c,II 114.75 K
c,II/c,I 231.8 K
c,I/liq 289.913 *K* $\Delta H = 11813$ J·mol^{-1}
$\Delta S = 40.75$ J·mol^{-1}·K^{-1}
Molecular Weight 133.1926
Wiswesser Line Notation T66 BNT&J
Evaluation A

$C_9H_{11}N$ (liq) 86STE/CHI2
5,6,7,8-Tetrahydroquinoline
Heat Capacity 298.15 K, $C_p = 217.33$ J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, $S = 248.69$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 222.634 K
Molecular Weight 133.1926
Wiswesser Line Notation T66 BN&TJ
Evaluation A

$C_9H_{11}N$ (liq) 89STE/CHI
5,6,7,8-Tetrahydroquinoline
Heat Capacity 298.15 K, $C_p = 217.41$ J·mol^{-1}·K^{-1}
Temperature range 5 to 440 K.
Entropy 298.15 K, $S = 248.73$ J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II *T*(glass) near 160 K
Glass to metastable form.
c,II/c,I near 210 K
First order transition, metastable to stable crystalline form.
c,I/liq 222.634 K $\Delta H = 9071.7$ J·mol^{-1}
$\Delta S = 40.75$ J·mol^{-1}·K^{-1}
Molecular Weight 133.1926
Wiswesser Line Notation T66 BN&TJ
Evaluation A

$C_9H_{12}O$ (liq) 88BAG/GUR
2,5,6-Trimethylphenol
Heat Capacity 298.15 K, $C_p = 224.7$ J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 136.1932
Wiswesser Line Notation QR B1 C1 F1
Evaluation B

$C_9H_{12}O_2$ (liq) 88BAG/GUR
Trimethylhydroquinone
Heat Capacity 313.65 K, C_p = 217.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 152.1926
Wiswesser Line Notation QR B1 C1 DQ E1
Evaluation B

$C_9H_{14}O$ (liq) 88BAG/GUR
2,5,6-Trimethyl-2-cyclohexen-1-one
Heat Capacity 298.15 K, C_p = 258.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 138.2090
Wiswesser Line Notation L6 BU CVTJ B1 E1 F1
Evaluation B

$C_9H_{14}O_2$ (liq) 85KAR/ABD2
Carbopropoxy methyl methacrylate
Phase Changes
c/liq 276.5 K, ΔH = 19867 J·mol^{-1}
Molecular Weight 154.2084
Wiswesser Line Notation 3OV1OVY1&U1
Evaluation A

$C_9H_{14}O_6$ (liq) 83RAB/KHL
Triacetin; Glycerol triacetate
Heat Capacity 300 K, C_p = 384.7 J·mol^{-1}·K^{-1}
Temperature range 9 to 320 K.
Entropy 300 K, S = 458.3 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 275.25 K, ΔH = 25800 J·mol^{-1}
ΔS = 93.8 J·mol^{-1}·K^{-1}
Molecular Weight 218.2060
Wiswesser Line Notation 1OV1YOV1&1OV1
Evaluation A
Data also given for vitreous and supercooled liquid states from 10 to 260 K. T(glass) = 198 K.

$C_9H_{14}O_6$ (liq) 86NIL/WAD
Triacetin
Heat Capacity 298.15 K, C_p = 389.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 218.2060
Wiswesser Line Notation 1VO1YOV1&1OV1
Evaluation A

$C_9H_{17}O_2Tl$ (c) 76MEI/SEY
Thallium nonanoate
Phase Changes
c,IV/c,III 300 K, ΔH = 1674 J·mol^{-1}
ΔS = 5.44 J·mol^{-1}·K^{-1}
c,III/c,II 315 K, ΔH = 2636 J·mol^{-1}
ΔS = 8.37 J·mol^{-1}·K^{-1}
c,II/c,I 330 K, ΔH = 7531 J·mol^{-1}
ΔS = 22.2 J·mol^{-1}·K^{-1}
liq/liq 490 K, ΔH = 2552 J·mol^{-1}
ΔS = 5.02 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,I/liq 410 K, ΔH = 5021 J·mol^{-1}
ΔS = 12.1 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 361.6021
Wiswesser Line Notation OV8 .TL
Evaluation B

$C_9H_{18}O$ (liq) 89VES/BAR
2,6-Dimethyl-4-heptanone; Diisobutylketone
Heat Capacity 298.15 K C_p = 297.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2406
Wiswesser Line Notation 1Y1&1V1Y1&1
Evaluation A

$C_9H_{18}O$ (liq) 70HAR/HEA
5-Nonanone
Heat Capacity 298.15 K, C_p = 303.0 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2406
Wiswesser Line Notation 4V4
Evaluation B

$C_9H_{18}O$ (liq) 82DYA/VAS
Nonanal; Pelargonaldehyde
Entropy 298.15 K, S = 397.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq ΔH = 30510 J·mol^{-1}
Molecular Weight 142.2406
Wiswesser Line Notation VH8
Evaluation B

C_9H_{20} (liq) 76FIN/MES
2,2,4,4-Tetramethylpentane
Heat Capacity 298.15 K, C_p = 266.3 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 331.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 206.61 K, ΔH = 9744.1 J·mol^{-1}
ΔS = 47.16 J·mol^{-1}·K^{-1}
Molecular Weight 128.2570
Wiswesser Line Notation 1X1&1&1X1&1&1
Evaluation A

C_9H_{20} (liq) 76FIN/MES
2,2,3,3-Tetramethylpentane
Heat Capacity 298.15 K, C_p = 271.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 334.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 174.45K, ΔH = 7325.45 J·mol^{-1}
ΔS = 41.99 J·mol^{-1}·K^{-1}
c,I/liq 263.40 K, ΔH = 2332.6 J·mol^{-1}
ΔS = 8.86 J·mol^{-1}·K^{-1}
Molecular Weight 128.2570
Wiswesser Line Notation 2X1&1&X1&1&1
Evaluation A

$C_9H_{18}O$ (liq) 84VAS/PET
Nonanal; Pelargonaldehyde
Heat Capacity 298.15 K, C_p = 290.26 J·mol^{-1}·K^{-1}
Temperature range 10 to 340 K.
Entropy 298.15 K, S = 396.97 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 253.83 K
Molecular Weight 142.2406
Wiswesser Line Notation VH8
Evaluation A

$C_9H_{18}O_2$ (liq) 84VAS/PET
Butyl pentanoic acid
Heat Capacity 300 K, C_p = 311.0 J·mol^{-1}·K^{-1}
Temperature range 190 to 370 K.
Phase Changes
c/liq 189.37 K, ΔH = 17600 J·mol^{-1}
ΔS = 92.94 J·mol^{-1}·K^{-1}
Molecular Weight 158.2400
Wiswesser Line Notation 4OV4
Evaluation A

$C_9H_{18}O_2$ (liq) 84VAS/PET
Amyl butyrate; Pentyl butanoate
Heat Capacity 300 K, C_p = 311.6 J·mol^{-1}·K^{-1}
Temperature range 200 to 370 K.
Phase Changes
c/liq 200.48 K, ΔH = 20010 J·mol^{-1}
ΔS = 99.81 J·mol^{-1}·K^{-1}
Molecular Weight 158.2400
Wiswesser Line Notation 5OV3
Evaluation A

$C_9H_{18}O_4$ (liq) 82BIR/SIK
2-(2′-Hydroxyethoxy)ethyl pivalate
Heat Capacity 298.15 K, C_p = 311.6 J·mol^{-1}·K^{-1}
Temperature range 270 to 370 K.
Equation only.
$C_p = 63.18 + 0.2288\ T + 0.002671\ T^2$ J·mol^{-1}·K^{-1}, (adjusted).
Molecular Weight 190.2388
Wiswesser Line Notation Q2O2OVX1&1&1
Evaluation C

C_9H_{20} (liq) 54STA/WAR
3,3-Diethylpentane; Tetraethylmethane
Heat Capacity 260 K, C_p = 260.9 J·mol^{-1}·K^{-1}
Temperature range 90 to 260 K.
Phase Changes
c,II/c,I 210.1 K, ΔH = 1272 J·mol^{-1}
Combined heats of transition for multiple phases.
c,I/liq 240.13 K, ΔH = 10033 J·mol^{-1}
ΔS = 47.82 J·mol^{-1}·K^{-1}
Combined entropies of fusion and transition.
Molecular Weight 128.2570
Wiswesser Line Notation 2X2&2&2
Evaluation B

C_9H_{20} (liq) 76FIN/MES
3,3-Diethylpentane; Tetraethylmethane
Heat Capacity 298.15 K, C_p = 278.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 333.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 208.25 K, ΔH = 483.7 J·mol^{-1}
ΔS = 2.32 J·mol^{-1}·K^{-1}
c,II/c,I 210.4 K, ΔH = 810.4 J·mol^{-1}
ΔS = 3.85 J·mol^{-1}·K^{-1}
c,I/liq 240.10 K, ΔH = 10089.7 J·mol^{-1}
ΔS = 42.02 J·mol^{-1}·K^{-1}
Molecular Weight 128.2570
Wiswesser Line Notation 2X2&2&2
Evaluation A

C_9H_{20} (liq) 82ZAR
n-Nonane
Heat Capacity 323 K, C_p = 293.2 J·mol^{-1}·K^{-1}
Temperature range 323, 363 K.
Molecular Weight 128.2570
Wiswesser Line Notation 9H
Evaluation B

$C_9H_{20}N_2O$ (c) 87DEL/FER
N,N′-Dibutylurea
Phase Changes
c,II/c,I 311.5 K, ΔH = 11100 J·mol^{-1}
ΔS = 35.6 J·mol^{-1}·K^{-1}
c/liq 346.9 K, ΔH = 14870 J·mol^{-1}
ΔS = 42.8 J·mol^{-1}·K^{-1}
Molecular Weight 172.2698
Wiswesser Line Notation 4MVM4
Evaluation A

$C_9H_{20}O_4$ (liq) 82ZAR
Tripropylene glycol
Heat Capacity 298 K, C_p = 440.6 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 192.2546
Wiswesser Line Notation QYOYOYQ
Evaluation B

$C_9H_{21}Al$ (liq) 84SHE/NIS
Tripropylaluminum
Heat Capacity 298.15 K, C_p = 340.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 370.1 J·mol^{-1}·K^{-1}
Molecular Weight 156.2464
Wiswesser Line Notation 3-AL-3&3
Evaluation A
T(glass) = 149.0 K.

$C_9H_{21}N_3O_6CaCl_2$ (c) 80LOP/TEL
Trisarcosine calcium chloride
Heat Capacity 300 K, C_p = 424 J·mol^{-1}·K^{-1}
Temperature range 50 to 330 K.
Data given graphically.
Value is an estimate from graph.
Phase Changes
c,II/c,I 130.27 K
Molecular Weight 378.2674
Wiswesser Line Notation QV1M1 3 .C*A* G2
Evaluation C

$C_9H_{24}Si_2$ (c) 75GUS/KAR
1,3-Bis(trimethylsilyl)propane
Heat Capacity 298.15 K, C_p = 394.34 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K. Data given graphically.
Entropy 298.15 K, S = 517.14 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 223.73 K, ΔH = 16058 J·mol^{-1}
ΔS = 71.76 J·mol^{-1}·K^{-1}
liq/g 444.52 K, ΔH = 43095 J·mol^{-1}
ΔS = 96.99 J·mol^{-1}·K^{-1}
Molecular Weight 188.4596
Wiswesser Line Notation 1-SI-1&1&3-SI-1&1&1
Evaluation B

$C_9H_{24}Si_3$ (c) 75GUS/KAR
1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane
Heat Capacity 298.15 K, C_p = 400.95 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Data given graphically.
Entropy 298.15 K, S = 477.39 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 269.28 K, ΔH = 16498 J·mol^{-1}
ΔS = 61.42 J·mol^{-1}·K^{-1}
liq/g 476.55 K, ΔH = 45522 J·mol^{-1}
ΔS = 95.52 J·mol^{-1}·K^{-1}
Molecular Weight 216.5451
Wiswesser Line Notation T6-SI- C-SI- E-SI-TJ
A1 A1 C1 C1 E1 E1
Evaluation B

$C_{10}D_{10}Fe$ (c) 83SHI/SOR
Ferrocene-d_{10}
Heat Capacity
Temperature range 13 to 300 K.
Data graphically only.
Phase Changes
c,III/c,II 164.1 K, $\Delta H = 878$ J·mol^{-1}
$\Delta S = 5.27$ J·mol^{-1}·K^{-1}
Lambda type transition in the metastable state.
c,II/c,I 251 K, $\Delta H = 4230$ J·mol^{-1}
$\Delta S = 16.83$ J·mol^{-1}·K^{-1}
Phase transition between stable LT and stable HT phases.
Molecular Weight 196.1150
Wiswesser Line Notation L5ØJ &1A-E/H-2 5Ø-FE--ØL5ØJ &1A-E/H-2 5
Evaluation A

$C_{10}D_{10}Fe$ (c) 84SOR/SHI
Ferrocene-d_{10}
Heat Capacity 298.15 K, $C_p = 221.94$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, $S = 233.18$ J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 164.1 K, $\Delta H = 878$ J·mol^{-1}
$\Delta S = 5.27$ J·mol^{-1}·K^{-1}
Lambda transition.
Secondary C_p maximum at 172 K.
c,II/c,I 251 K, $\Delta H = 4230$ J·mol^{-1}
$\Delta S = 16.83$ J·mol^{-1}·K^{-1}
Molecular Weight 196.1150
Wiswesser Line Notation L5ØJ &1A-E/H-2 5Ø-FE--ØL5ØJ &1A-E/H-2 5
Evaluation A
Data also given for the metastable phases over temperature range 10 to 250 K.

$C_{10}H_2O_6$ (c) 77KAR/BAZ
Pyromellitic dianhydride
Heat Capacity 300 K, $C_p = 219.9$ J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, $S = 242.1$ J·mol^{-1}·K^{-1}
Molecular Weight 218.1222
Wiswesser Line Notation T565 DVOV JVOVJ
Evaluation B

$C_{10}H_5Cu$ (c) 82BYK/LEB
Copper phenylethynylacetylenide
Heat Capacity 298.15 K, $C_p = 184.4$ J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, $S = 202.7$ J·mol^{-1}·K^{-1}
Molecular Weight 188.6955
Wiswesser Line Notation -CU-1UU2UU1R
Evaluation A

$C_{10}H_7Cl$ (liq) 81GRO/ING
1-Chloronaphthalene
Heat Capacity 298.15 K, $C_p = 211.37$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.6183
Wiswesser Line Notation L66J BG
Evaluation B

$C_{10}H_7Cl$ (liq) 86WIL/LAI
1-Chloronaphthalene
Heat Capacity 298.15 K, $C_p = 211.28$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 162.6183
Wiswesser Line Notation L66J BG
Evaluation B

$C_{10}H_7Cl$ (c) 78LOY/REY
2-Chloronaphthalene
Heat Capacity 250 K, $C_p = 150$ J·mol^{-1}·K^{-1}
Temperature range 4.2 to 300 K.
Data given graphically and estimated from graph.
Transition at 308 K makes heat capacity at 298 K anomalous.
Phase Changes
c,III/c,II 12 K
Anomalous transition.
c,II/c,I 308 K
Anomalous transition.
Molecular Weight 162.6183
Wiswesser Line Notation L66J CG
Evaluation D(C_p); C(Phase changes)

$C_{10}H_7F$ (c) 78LOY/REY
2-Fluoronaphthalene
Heat Capacity 250 K, $C_p = 190$ J·mol^{-1}·K^{-1}
Temperature range 4.2 to 300 K.
Data given graphically and estimated from graph.
Transition at 277 K makes heat capacity at 298 K anomalous.
Phase Changes
c,IV/c,II 161 K
Anomalous transition; sharp peak.
c,III/c,II 240 K
Anomalous transition.
c,II/c,I 277 K
Anomalous transition.
c,I/liq 331 K
Molecular Weight 146.1637
Wiswesser Line Notation L66J CF
Evaluation D(C_p); C(Phase changes)

$C_{10}H_8$ (c) 82SYU/TUM
Naphthalene
Phase Changes
c/liq 354.1 K, $\Delta H = 19020$ J·mol^{-1}
$\Delta S = 53.7$ J·mol^{-1}·K^{-1}
Relative error in determination ± 5%.
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation C

$C_{10}H_8$ (c) 88TOR/BAR
Naphthalene
Phase Changes
liq/g 323 K, $\Delta H = 70850$ J·mol^{-1}
$\Delta S = 219.3$ J·mol^{-1}·K^{-1}
c/g 298.15 K, $\Delta H = 72320$ J·mol^{-1}
$\Delta S = 242.6$ J·mol^{-1}·K^{-1}
Molecular Weight 128.1732
Wiswesser Line Notation L66J
Evaluation A

$C_{10}H_8Cl$ (liq) 88COS/HUU
1-Chloronaphthalene
Heat Capacity 298.15 K, $C_p = 212.60$ J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 163.6262
Wiswesser Line Notation L66J BG
Evaluation B

$C_{10}H_{10}$ (c) 80FAL
Bullvalene; Tricyclo[3.3.2.0^{4,6}]deca-2,7,9-triene
Heat Capacity 298.15 K, C_p = 190.38 J·mol^{-1}·K^{-1}
Temperature range 5 to 450 K.
Entropy 298.15 K, S = 174.66 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 366.5 K, ΔH = 15250 J·mol^{-1}
ΔS = 41.61 J·mol^{-1}·K^{-1}
Molecular Weight 130.1890
Wiswesser Line Notation L737 B C 1A J BU EU IUTJ
Evaluation A

$C_{10}H_{10}$ (liq) 49PAR/HAT
cis-Decahydronaphthalene
Heat Capacity 298.15 K, C_p = 220.06 J·mol^{-1}·K^{-1}
Temperature range 80 to 298.15 K.
Phase Changes
c/liq 230.1 K, ΔH = 2209 J·mol^{-1}
ΔS = 9.6 J·mol^{-1}·K^{-1}
Molecular Weight 130.1890
Wiswesser Line Notation L66TTJ -C
Evaluation B

$C_{10}H_{10}$ (liq) 49PAR/HAT
trans-Decahydronaphthalene
Heat Capacity 298.15 K, C_p = 217.72 J·mol^{-1}·K^{-1}
Temperature range 80 to 298.15 K.
Phase Changes
c/liq 242.4 K, ΔH = 3244 J·mol^{-1}
ΔS = 13.4 J·mol^{-1}·K^{-1}
Molecular Weight 130.1890
Wiswesser Line Notation L66TTJ -T
Evaluation B

$C_{10}H_{10}Co$ (c) 75RAB/NIS
Cobaltocene
Heat Capacity 298.15 K, C_p = 197.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S = 236.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 92 K, ΔH = 238 J·mol^{-1}
ΔS = 2.73 J·mol^{-1}·K^{-1}
Lambda transition between 70 to 140 *K* with a maximum at 92 K.
Molecular Weight 189.1222
Wiswesser Line Notation L5ØJ Ø-CO-- ØL5ØJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Co$ (c) 76POM/AZO
Cobaltocene
Heat Capacity 298.15 K
Temperature range 118 to 298 K. Data given graphically.
C_p=62.92–0.460T+6.07×10$^{-3}T^2$–9.53×10$^{-6}T^3$ (118 to 298 K).
C_p value calculated from equation.
Molecular Weight 189.1222
Wiswesser Line Notation L5ØJ Ø-CO-- ØLTØJ
Evaluation C

$C_{10}H_{10}Cr$ (c) 75RAB/NIS
Chromocene
Heat Capacity 298.15 K, C_p = 199.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S = 236.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 99.5 K, ΔH = 265 J·mol^{-1}
ΔS = 2.57 J·mol^{-1}·K^{-1}
Lambda transition between 75 to 140 K with a maximum at 99.7 K and another flat peak at 118 K.
Molecular Weight 182.1850
Wiswesser Line Notation L5ØJ Ø-CR-- ØL5ØJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Cr$ (c) 76POM/AZO
Chromocene
Heat Capacity 298.15 K
Temperature range 121 to 298 K.
Data given graphically.
C_p = −253.6 + 0.632T + 33.52×10$^3T^{-1}$ J·mol^{-1}·K^{-1}. (213 to 298 K).
Phase Changes
c,II/c,I 160–230 K, ΔS = 1.5 J·mol^{-1}·K^{-1}
Lambda type transition.
Molecular Weight 182.1850
Wiswesser Line Notation L5ØJ Ø-CR-- ØL5ØJ
Evaluation C(C_p), A(Phase changes)

$C_{10}H_{10}Cr$ (c) 84CHH/POM
Chromocene
Heat Capacity 298 K, C_p = 198.5 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Unsmoothed experimental datum.
Molecular Weight 182.1850
Wiswesser Line Notation L5ØJ Ø-CR-- ØL5ØJ
Evaluation B
Lambda anomaly at 100 K.

$C_{10}H_{10}F_6FeP$ (c) 86SOR/SHI
Ferrocenium hexafluorophosphate
Heat Capacity
Temperature range 12 to 393 K.
Data given graphically.
Phase Changes
c,IV/c,III 210.95 K
c,III/c,II 213.05 K, ΔH = 1950 J·mol^{-1}
ΔS = 9.54 J·mol^{-1}·K^{-1}
ΔH and ΔS are total of c,IV/c,III and c,III/c,II transitions.
c,II/c,I 346.94 K, ΔH = 4840 J·mol^{-1}
ΔS = 13.99 J·mol^{-1}·K^{-1}
Molecular Weight 331.0002
Wiswesser Line Notation L5ØJ Ø-FE-- ØL5ØJ &PFFFFFF
Evaluation A

$C_{10}H_{10}Fe$ (c) 76POM/AZO
Ferrocene
Heat Capacity
Temperature range 120 to 200 K.
Data given graphically.
Phase Changes
c,II/c,I 164 K, ΔH = 853 J·mol^{-1}
ΔS = 5.31 J·mol^{-1}·K^{-1}
Molecular Weight 186.0360
Wiswesser Line Notation L5ØJ Ø-FE-- ØL5ØJ
Evaluation A

$C_{10}H_{10}Mn$ (c) 75RAB/NIS
Manganocene
Heat Capacity 298.15 K, C_p = 208.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S = 251.4 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 55–75 K, ΔH = 41 J·mol^{-1}
ΔS = 0.63 J·mol^{-1}·K^{-1}
Lambda transition.
Molecular Weight 185.1270
Wiswesser Line Notation L5ØJ Ø-MN- - ØL5ØJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}N_2O_2$ (c) 82CUE/SOL
N-Ethanol isatoxine
Phase Changes
c/liq 505 K, ΔH = 28900 J·mol^{-1}
ΔS = 57.2 J·mol^{-1}·K^{-1}
Molecular Weight 190.2012
Wiswesser Line Notation T56 BMVHJ DUNO2
Evaluation D

$C_{10}H_{10}Ni$ (c) 75RAB/NIS
Nickelocene
Heat Capacity 298.15 K, C_p = 205.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S = 253.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 100–190 K, ΔH = 182 J·mol^{-1}
ΔS = 1.32 J·mol^{-1}·K^{-1}
Lambda transition.
Molecular Weight 188.8890
Wiswesser Line Notation L5ØJ Ø-NI- - ØL5ØJ
Evaluation A
See also 78RAB/NIS.

$C_{10}H_{10}Ni$ (c) 76POM/AZO
Nickelocene
Heat Capacity 298.15 K
Temperature range 127 to 303 K.
Data given graphically.
$C_p = 87.705 - 0.649T + 5.86\times10^{-3}T^2 - 9.29\times10^{-6}T^3$ J·mol^{-1}·K^{-1} (127 to 170 K: 240 to 303 K).
C_p value calculated from equation.
Phase Changes
c,II/c,I 170–240 K, ΔS = 5.2 J·mol^{-1}·K^{-1}
Molecular Weight 188.8890
Wiswesser Line Notation L5ØJ Ø-NI- - ØL5ØJ
Evaluation $C(C_p)$, A(Phase changes)

$C_{10}H_{10}O_2$ (c) 84BEK/RUE
Homocubane-4-carboxylic acid;
4-Carboxypentacyclo[4.3.0.0^{2,5}.0^{3,8}.0^{4,7}]nonane
Heat Capacity 298 K, C_p = 207 J·mol^{-1}·K^{-1}
C_p given as 0.305 cal·K^{-1}·g^{-1}.
Phase Changes
liq/g ΔH = 82006 J·mol^{-1}
ΔH from 80DUC/GRU.
Molecular Weight 162.1878
Wiswesser Line Notation L444 B4 D5 4ABCD ITJ AVQ
Evaluation B

$C_{10}H_{10}O_4$ (liq) 70MAR/RAB
Dimethyl *o*-phthalate
Heat Capacity 300 K, C_p = 303.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S = 365.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 274.18 K, ΔH = 16945 J·mol^{-1}
ΔS = 61.8 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation B
See also 69RAB/MAR. T(glass) = 192.0 °C.

$C_{10}H_{10}O_4$ (liq) 84VAS/PET
Dimethyl-o-phthalate
Heat Capacity 300 K, C_p = 303.8 J·mol^{-1}·K^{-1}
Temperature range 25 to 360 K.
Entropy 300 K, S = 365.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 274.18 K
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation A

$C_{10}H_{10}O_4$ (liq) 86RAB/NOV
Dimethyl-o-phthalate
Heat Capacity 298.15 K, C_p = 303.1 J·mol^{-1}·K^{-1}
Temperature range 6 to 120 K.
Entropy 298.15 K, S = 353.9 J·mol^{-1}·K^{-1}
Molecular Weight 194.1866
Wiswesser Line Notation 1OVR BVO1
Evaluation A
Low temperature study of vitreous and crystalline forms.
Thermodynamic functions calculated for temperature range 0 to 360 K.

$C_{10}H_{10}Ru$ (c) 76POM/AZO
Ruthenocene
Heat Capacity 298.15 K
Temperature range 100 to 300 K.
Data given graphically.
$C_p = 74.33 + 2.59T - 1.50\times10^{-3}T^2 + 2.31\times10^{-5}T^3 - 4.35\times10^{-8}T^4$ J·mol^{-1}·K^{-1} (100 to 300K).
Molecular Weight 231.2590
Wiswesser Line Notation L5ØJ Ø-RU- - ØL5ØJ
Evaluation C

$C_{10}H_{10}V$ (c) 75RAB/NIS
Vanadocene
Heat Capacity 298.15 K, C_p = 204.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 298.15 K.
Entropy 298.15 K, S = 340.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 130–200 K, ΔH = 196 J·mol^{-1}
ΔS = 1.21 J·mol^{-1}·K^{-1}
Lambda transition.
Molecular Weight 181.1305
Wiswesser Line Notation L5ØJ Ø-VA- - ØL5ØJ
Evaluation A

$C_{10}H_{12}$ (c) 77LEB/LIT4
endo-Dicyclopentadiene
Heat Capacity 298.15 K, C_p = 188.7 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S = 230.0 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 216 K, ΔH = 9660 J·mol^{-1}
ΔS = 40.0 J·mol^{-1}·K^{-1}
c,I/liq 304.8 K, ΔH = 2220 J·mol^{-1}
ΔS = 6.1 J·mol^{-1}·K^{-1}
Molecular Weight 132.2048
Wiswesser Line Notation L C555 A EU IUTJ -C
Evaluation A

$C_{10}H_{12}N_2O_3$ (c) 82CUE/SOL
2-Ethoxyisonitrosoacetanilide
Phase Changes
c/liq 405 K, ΔH = 23000 J·mol^{-1}
ΔS = 56.8 J·mol^{-1}·K^{-1}
Molecular Weight 208.2164
Wiswesser Line Notation QNU1VMR BO2
Evaluation D

$C_{10}H_{12}N_2O_3$ (c) 82CUE/SOL
4-Ethoxyisonitrosoacetanilide
Phase Changes
c/liq 490 K, ΔH = 7600 J·mol^{-1}
ΔS = 15.5 J·mol^{-1}·K^{-1}
Molecular Weight 208.2164
Wiswesser Line Notation QVU1MR DO2
Evaluation D

$C_{10}H_{12}O_2$ (liq) 83KAR/ABD
Eugenol; 5-Allylguaiacol
Heat Capacity 293 K, C_p = 343.2 J·mol^{-1}·K^{-1}
Temperature range 243 to 293 K.
C_p given as 2090 J·kg^{-1}·K^{-1}.
Molecular Weight 164.2036
Wiswesser Line Notation QR B01 D2U1
Evaluation B

$C_{10}H_{12}N_2S$ (c) 28SHI
N-Allyl-N'-phenylthiourea
Heat Capacity 323 K, C_p = 59.0 J·mol^{-1}·K^{-1}
Temperature range:
C_p measured at 50°, 70 °C, 99.8 °C.
Phase Changes
c/liq 375 K, ΔH = 27614 J·mol^{-1}
ΔS = 73.6 J·mol^{-1}·K^{-1}
Molecular Weight 192.2782
Wiswesser Line Notation 1U2MYMUS&R
Evaluation B

$C_{10}H_{14}Si$ (liq) 77LEB/RAB2
Vinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p = 284.8 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S = 374.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.70 K, ΔH = 12259 J·mol^{-1}
ΔS = 64.4 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation 1U1-SI-1&1&R
Evaluation A
T(glass) = 129.5 K.

$C_{10}H_{14}Si$ (liq) 81LEB/LEB
Vinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p = 284.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 374.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 190.70 K, ΔH = 12300 J·mol^{-1}
ΔS = 64.4 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation 1U1-SI-1&1&R
Evaluation A
T(glass) = 129 K.

$(C_{10}H_{14}Si)_n$ (c) 75LEB/ARO
Polyvinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p = 231.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S = 247.2 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*1Y*-SI-1&1&R/
Evaluation B

$(C_{10}H_{14}Si)_n$ (c) 81LEB/LEB
Polyvinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p = 231.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 247.2 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*1Y*-SI-1&1&R/
Evaluation A

$(C_{10}H_{14}Si)_n$ (gls) 77LEB/RAB2
Polyvinyldimethylphenylsilane
Heat Capacity 298.15 K, C_p = 231.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 300 K.
Entropy 298.15 K, S = 247.2 J·mol^{-1}·K^{-1}
Molecular Weight 162.3061
Wiswesser Line Notation /*1Y*-SI-1&1&R/
Evaluation A

$C_{10}H_{14}ZnO_4$ (c) 86GRI/LAZ
Zinc acetylacetonate
Phase Changes
c/liq 400.5 K, ΔH = 18200 J·mol^{-1}
ΔS = 45.5 J·mol^{-1}·K^{-1}
Molecular Weight 263.5982
Wiswesser Line Notation D6O-ZN-O ADJ D1 F1
B-& BD6O-ZN-O ADJ D1 F1
Evaluation A

$C_{10}H_{15}Cl$ (c) 88PAR/KAW
2-Chloroadamantane
Phase Changes
c,III/c,II 227 K, ΔH = 470 J·mol^{-1}
ΔS = 2.3 J·mol^{-1}·K^{-1}
c,II/c,I 242 K, ΔH = 8300 J·mol^{-1}
ΔS = 35 J·mol^{-1}·K^{-1}
Molecular Weight 170.6815

Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ AG
Evaluation A

$C_{10}H_{16}$ (liq) 78GOO/SCO
exo-Tetrahydrodicyclopentadiene
Heat Capacity 298.15 K, C_p = 236.50 J·mol^{-1}·K^{-1}
Temperature range 275 to 365 K.
Equation only.
C_p calculated from equation.
C_s = 0.046061 + 0.0012371 T cal·g^{-1}·K^{-1} (275 to 365 K).
Molecular Weight 136.2364
Wiswesser Line Notation L C555 ATJ -T
Evaluation B

$C_{10}H_{16}$ (liq) 79SMI/GOO
exo-Tetrahydrodicyclopentadiene
Heat Capacity 298.15 K, C_p = 236.6 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.415 cal·K^{-1}·g^{-1}.
Molecular Weight 136.2364
Wiswesser Line Notation L C555 ATJ -T
Evaluation B

$C_{10}H_{16}$ (liq) 80GOO/THO
exo-Tetrahydrodicyclopentadiene
Heat Capacity 298.15 K, C_p = 213.87 J·mol^{-1}·K^{-1}
Temperature range 260 to 465 K. Equation only.
C_p calculated from equation C_p (cal·K^{-1}·g^{-1}) = 0.10423 + 0.76872×10^{-3} T + 0.46992×10^{-6} T^2 (260 to 465 K).
Molecular Weight 136.2364
Wiswesser Line Notation L C555 ATJ -T
Evaluation B

$C_{10}H_{16}N_2ClO_4$ (c) 65CHI/NAK
Wurster's Blueperchlorate; N,N,N',N'-Tetramethyl-*p*-phenylene-diamine perchlorate
Heat Capacity 200 K, C_p = 264 J·mol^{-1}·K^{-1}
Temperature range 80 to 200 K.
Data graphically only and estimated from graph.
Phase Changes
c,II/c,I 189.9 K, ΔH = 1709.6 J·mol^{-1}
ΔS = 9.16 J·mol^{-1}·K^{-1}
Transition is probably first-order.
Molecular Weight 263.7004
Wiswesser Line Notation 1N1&R DN1&1 &GWW
Evaluation A

$C_{10}H_{16}O$ (liq) 88BAG/GUR
3,7-Dimethyl-6-octen-1-yn-3-ol
Heat Capacity 313.55 K, C_p = 385.2 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 152.2358
Wiswesser Line Notation 1YU3XQ1UU1
Evaluation B

$C_{10}H_{16}O$ (c) 88SAL/ABA
1-Hydroxyadamantane
Phase Changes
c,III/c,II 369.16 K, ΔH = 2500 J·mol^{-1}
ΔS = 6.77 J·mol^{-1}·K^{-1}
c,II/c,I 529.16 K, ΔH = 7130 J·mol^{-1}
ΔS = 13.25 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ FQ
Evaluation A

$C_{10}H_{16}O$ (c) 88SAL/ABA
2-Hydroxyadamantane
Phase Changes
c,IV/c,III 325.16 K, ΔH = 300 J·mol^{-1}
ΔS = 0.92 J·mol^{-1}·K^{-1}
c,III/c,II 391.16 K, ΔH = 3740 J·mol^{-1}
ΔS = 9.56 J·mol^{-1}·K^{-1}
c,II/c,I 516.16 K, ΔH = 7750 J·mol^{-1}
ΔS = 15.02 J·mol^{-1}·K^{-1}
Molecular Weight 152.2358
Wiswesser Line Notation L66 B6 /B-H/ A B- C 1B ITJ AQ
Evaluation A

$C_{10}H_{16}O$ (liq) 82KAR/IGA
Citral; Geranial
Heat Capacity 293 K, C_p = 304.5 J·mol^{-1}·K^{-1}
Temperature range 233 to 293 K.
C_p given as 2000 J·kg^{-1}·K^{-1}.
Molecular Weight 152.2358
Wiswesser Line Notation VHOYUY1&3UY1&1
Evaluation B

$(C_{10}H_{16}O_4)_n$ (c) 84RAB/NIS
Polybutylene glycol adipate
Heat Capacity 298.15 K, C_p = 316.7 J·mol^{-1}·K^{-1}
Temperature range 80 to 470 K.
100% crystallinity.
C_p(298.15 K) = 393.6 J·mol^{-1}·K^{-1} for the highly elastic state.
Entropy 298.15 K, S = 334.9 J·mol^{-1}·K^{-1}
100% crystallinity.
S°(298.15) − S°(0) = 379.9 J·mol^{-1}·K^{-1} for the highly elastic state.
Phase Changes
c/liq 328.8 K, ΔH = 24800 J·mol^{-1}
Molecular Weight 200.2340
Wiswesser Line Notation /*OV4VO4*/
Evaluation B
T(glass) = 199 K.

$C_{10}H_{18}$ (liq) 88SHI/OGA
cis-Decahydronaphthalene; *cis*-Decalin
Heat Capacity 298.15 K, C_p = 232.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation A

$C_{10}H_{18}$ (liq) 88SHI/OGA2
cis-Decahydronaphthalene; *cis*-Decalin
Heat Capacity 298.15 K, C_p = 232.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -C
Evaluation A

$C_{10}H_{18}$ (liq) 88SHI/OGA
trans-Decahydronaphthalene; *trans*-Decalin
Heat Capacity 298.15 K, C_p = 229.17 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 138.2522
Wiswesser Line Notation L66TJ -T
Evaluation A

$C_{10}H_{18}$ (liq) 88SHI/OGA2

trans-Decahydronaphthalene; *trans*-Decalin

Heat Capacity 298.15 K, C_p = 229.17 J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 138.2522

Wiswesser Line Notation L66TJ -T

Evaluation A

$C_{10}H_{18}O_4$ (liq) 86NIL/WAD

Ethyleneglycol dibutanoate

Heat Capacity 298.15 K, C_p = 380.3 J·mol^{-1}·K^{-1}

One temperature.

Molecular Weight 202.2498

Wiswesser Line Notation 3VO2OV3

Evaluation A

$C_{10}H_{19}NO_2$ (liq) 85KAR/ABD2

Diethylaminoethyl methacrylate

Phase Changes

c/liq 207.5 K, ΔH = 13080 J·mol^{-1}; ΔS = 63.04 J·mol^{-1}·K^{-1}

Molecular Weight 185.2656

Wiswesser Line Notation 1UY1&VO2N2&2

Evaluation A

$C_{10}H_{19}O_2Tl$ (c) 88LOP/CHE

Thallium (I) *n*-decanoate

Heat Capacity 300 K, C_p = 426.5 J·mol^{-1}·K^{-1}

Temperature range 6 to 480 K.

Entropy 300 K, S = 403.3 J·mol^{-1}·K^{-1}

Phase Changes

c,V/c,IV 232.4 K, ΔH = 2411 J·mol^{-1}; ΔS = 10.39 J·mol^{-1}·K^{-1}

c,IV/c,III 288.6 K, ΔH = 599 J·mol^{-1}; ΔS = 2.08 J·mol^{-1}·K^{-1}

c,III/c,II 306.8 K, ΔH = 4240 J·mol^{-1}; ΔS = 13.89 J·mol^{-1}·K^{-1}

c,II/c,I 327.4 K, ΔH = 3974 J·mol^{-1}; ΔS = 12.14 J·mol^{-1}·K^{-1}

c,I/liq 405.0 K, ΔH = 5670 J·mol^{-1}; ΔS = 13.97 J·mol^{-1}·K^{-1}

Solid-mesophase.

liq/liq 484.0 K, ΔH = 2552 J·mol^{-1}; ΔS = 5.24 J·mol^{-1}·K^{-1}

Mesophase-isotropic liquid.

Molecular Weight 375.6289

Wiswesser Line Notation OV9 .TL

Evaluation A

$C_{10}H_{20}$ (c) 80BYS

2,2,5,5-Tetramethylhex-3-ene

Phase Changes

c,III/c,II 235.7 K, ΔH = 1210 J·mol^{-1}; ΔS = 5.13 J·mol^{-1}·K^{-1}

c,II/c,I 243.5 K, ΔH = 4330 J·mol^{-1}; ΔS = 17.8 J·mol^{-1}·K^{-1}

c,I/liq 268.8 K, ΔH = 10250 J·mol^{-1}; ΔS = 38.1 J·mol^{-1}·K^{-1}

Molecular Weight 140.2688

Wiswesser Line Notation 1X1&1&1U1X1&1&1

Evaluation A

$C_{10}H_{20}BrFeN_2S_4$ (c) 83YOS/SOR

Bromo bis(N,N-diethyldithiocarbamate)iron (III)

Heat Capacity 298.095 K, C_p = 434.5 J·mol^{-1}·K^{-1}

Temperature range 0.4 to 393 K.

Unsmoothed experimental datum.

Phase Changes

c,IV/c,III 1.347 K

Lambda type ferromagnetic transition.

c,III/c,II 9 K, ΔH = 97.0 J·mol^{-1}; ΔS = 11.05 J·mol^{-1}·K^{-1}

Schottky type anomaly.

ΔH and ΔS values are the total of both transitions.

c,II/c,I 265.7 K, ΔH = 1960 J·mol^{-1}; ΔS = 7.51 J·mol^{-1}·K^{-1}

Non−magnetic phase transition.

Molecular Weight 432.2724

Wiswesser Line Notation SUYS&N2&2 2 .FE E

Evaluation A(Phase changes), C(C_p)

Values given for sample A. (see text)

$C_{10}H_{20}O$ (liq) 80DYA/VAS

Decanal; Capric aldehyde; Capraldehyde

Heat Capacity

Temperature range 50 to 350 K.

Phase Changes

c/liq 269.47 K, ΔH = 30600 J·mol^{-1}; ΔS = 113.6 J·mol^{-1}·K^{-1}

97.10 mol% purity.

Molecular Weight 156.2674

Wiswesser Line Notation VH9

Evaluation B

Manuscript deposited in Cent. Sci. Res. Inst. Tech. Eng. Petrochemicals, July 27, 1979.

$C_{10}H_{20}O$ (liq) 82DYA/VAS

Decanal; Capric aldehyde; Capraldehyde

Entropy 298.15 K, S = 429.5 J·mol^{-1}·K^{-1}

Phase Changes

c/liq ΔH = 34500 J·mol^{-1}

Molecular Weight 156.2674

Wiswesser Line Notation VH9

Evaluation B

$C_{10}H_{20}O$ (liq) 84VAS/PET

Decanal; Capric aldehyde; Capraldehyde

Heat Capacity 298.15 K, C_p = 319.67 J·mol^{-1}·K^{-1}

Temperature range 10 to 337.5 K.

Entropy 298.15 K, S = 429.46 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 269.25 K

Molecular Weight 156.2674

Wiswesser Line Notation VH9

Evaluation A

$C_{10}H_{20}O_2$ (c) 1889EYK

Decanoic acid; Capric acid

Phase Changes

c/liq 300.1 K, ΔH = 29217 J·mol^{-1}; ΔS = 97.4 J·mol^{-1}·K^{-1}

Molecular Weight 172.2668

Wiswesser Line Notation QV9

Evaluation C

$C_{10}H_{22}$ (liq) 82ZAR

n-Decane

Heat Capacity 298 K, C_p = 312.8 J·mol^{-1}·K^{-1}

Temperature range 298, 323, 363 K.

Molecular Weight 142.2838

Wiswesser Line Notation 10H

Evaluation B

$C_{10}H_{22}$ (liq) 84GRO/ING
n-Decane
Heat Capacity 298.15 K, C_p = 313.93 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 84ROU/GRO
n-Decane
Heat Capacity 298.15 K, C_p = 314.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85LAI/ROU
n-Decane
Heat Capacity 298.15 K, C_p = 313.09 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 85LAI/WIL
n-Decane
Heat Capacity 298.15 K, C_p = 313.09 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}$ (liq) 86GAT/WOO
n-Decane
Heat Capacity 298.15 K, C_p = 313.56 J·mol^{-1}·K^{-1}
Temperature range 298.15 to 368.15 K.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation C

$C_{10}H_{22}$ (liq) 86TAR/AIC
n-Decane
Heat Capacity 298.15 K, C_p = 315.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 88COS/HUU
n-Decane
Heat Capacity 298.15 K, C_p = 315.32 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation B

$C_{10}H_{22}$ (liq) 88PER/AIC
n-Decane
Heat Capacity 298.15 K, C_p = 313.46 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 142.2838
Wiswesser Line Notation 10H
Evaluation A

$C_{10}H_{22}N_4$ (liq) 88BOB/KAM
Dipiperazinylethane
Heat Capacity 413 K, C_p = 540 J·mol^{-1}·K^{-1}
Temperature Range 413 to 473 K
Molecular Weight 174.2886
Wiswesser Line Notation T6M DNTJ D2- DT6M DNTJ
Evaluation D

$C_{10}H_{25}N_5$ (liq) 88BOB/KAM
N-(2-Aminoethyl)-N'-[(2-aminoethyl)2-aminoethyl]piperazine
Heat Capacity 333 K, C_p = 529 J·mol^{-1}·K^{-1}
Temperature Range 333 to 473 K
Molecular Weight 191.3190
Wiswesser Line Notation T6N DNTJ A2M2Z D2Z
Evaluation D

$C_{10}H_{22}S$ (liq) 82TUT/GAB
1-Decanethiol; *n*-Decyl mercaptan
Heat Capacity 300 K, C_p = 365.44 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 346.70 + 3.600\times10^{-2}T + 8.824\times10^{-5}T^2$.
Molecular Weight 174.3438
Wiswesser Line Notation SH10
Evaluation B

$C_{10}H_{24}ClN$ (c) 88VAN/WHI
Di-*n*-pentylammonium chloride
Heat Capacity 296.32 K, C_p = 353.9 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 243.84 K, ΔH = 1312.5 J·mol^{-1}
ΔS = 5.38 J·mol^{-1}·K^{-1}
Molecular Weight 193.7593
Wiswesser Line Notation 5M5 &GH
Evaluation A

$C_{10}H_{24}CuN_6O_6$ (c) 80CLA/STE
Cyclam; 1,4,8,11-Tetraazacyclotetradecane
Heat Capacity 298.15 K, C_p = 374.61 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.87 J·g^{-1}·K^{-1}.
Molecular Weight 200.3264
Wiswesser Line Notation T14M DM HM KMTJ
Evaluation B

$C_{10}H_{24}N_4{\cdot}Cu(NO_3)_2$ (c) 80CLA/STE
Bis(nitrato)(1,4,8,11-tetraazacyclotetradecane); copper (II);
1,4,8,11-Tetraazacyclotetradecane copper (II) nitrate
Heat Capacity 298.15 K, C_p = 915.40 J·mol^{-1}·K^{-1}
One temperature. C_p given as 2.36 J·g^{-1}·K^{-1}.
Molecular Weight 387.8822
Wiswesser Line Notation T14M DM HM KMTJ &.CU..N-O3*2
Evaluation B

$C_{10}H_{26}O_3Si_3$ (liq) 87DZH/KUL3
1,1,3,3-Tetraethyl-5,5-dimethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p = 502.8 J·mol^{-1}·K^{-1}
Temperature range 5 to300 K.
Entropy 298.15 K, S = 616.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 195–210 K, ΔH = 131 J·mol^{-1}
ΔS = 0.946 J·mol^{-1}·K^{-1}
c,I/liq 260.03 K, ΔH = 9522 J·mol^{-1}
ΔS = 36.75 J·mol^{-1}·K^{-1}
Molecular Weight 278.5701
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E1 E1
Evaluation A

$C_{10}H_{28}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(pentylammonium) manganese II
Phase Changes

c,IV/c,III	203 K,	ΔH = 53.2 J·mol^{-1}
		ΔS = 0.26 J·mol^{-1}·K^{-1}
c,III/c,II	208 K,	ΔH = 506.8 J·mol^{-1}
		ΔS = 2.43 J·mol^{-1}·K^{-1}
c,II/c,I	364 K,	ΔH = 3.6 J·mol^{-1}
		ΔS = 0.009 J·mol^{-1}·K^{-1}

Molecular Weight 373.0946
Wiswesser Line Notation 5ZH 2 .MN G4
Evaluation A

$C_{10}H_{28}Cl_4N_2Zn$ (c) 84CUE/TEL
Bis-pentylammonium tetrachloro zincate
Heat Capacity 300 K, C_p = 518.27 J·mol^{-1}·K^{-1}
Temperature range 55 to 355 K.
Entropy 300 K, S = 525.82 J·mol^{-1}·K^{-1}
Phase Changes

c,V/c,IV	141.5 K,	ΔH = 441 J·mol^{-1}
		ΔS = 3.08 J·mol^{-1}·K^{-1}
c,IV/c,III	147.95 K,	ΔH = 499 J·mol^{-1}
		ΔS = 3.33 J·mol^{-1}·K^{-1}
c,III/c,II	249.95 K,	ΔH = 3584 J·mol^{-1}
		ΔS = 14.38 J·mol^{-1}·K^{-1}
c,II/c,I	349.05 K,	ΔH = 8672 J·mol^{-1}
		ΔS = 24.36 J·mol^{-1}·K^{-1}
c,I/liq	437 K,	ΔH = 6800 J·mol^{-1}

Solid-isotropic liquid.
Molecular Weight 383.5366
Wiswesser Line Notation 5ZH 2 .ZN G4

$C_{11}H_{10}O_4$ (c) 84LEB/LEB
p-Methacryloyloxybenzoic acid
Heat Capacity 298.15 K, C_p = 257.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S = 284.1 J·mol^{-1}·K^{-1}
Phase Changes

c/liq	455 K,	ΔH = 34000 J·mol^{-1}
		ΔS = 75 J·mol^{-1}·K^{-1}

Molecular Weight 206.1976
Wiswesser Line Notation QVR DOVY1&U1
Evaluation A

$(C_{11}H_{10}O_4)_n$ (gls) 84LEB/LEB
Poly-p-methyacryloyloxybenzoic acid
Heat Capacity 298.15 K, C_p = 258.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, S = 261.5 J·mol^{-1}·K^{-1}
Molecular Weight 206.1976
Wiswesser Line Notation /*X1*&1&VOR DVQ/
Evaluation A
T(glass) = 316 K.

$C_{11}H_{11}F_6FeP$ (c) 86SOR/SHI
(Cyclohexatriene)(cyclopentadienyl)iron(II) hexafluorophosphate
Heat Capacity
Temperature range 12 to 393 K.
Data given graphically.
Phase Changes

c,V/c,IV	158.3 K,	ΔH = 1190 J·mol^{-1}
		ΔS = 8.01 J·mol^{-1}·K^{-1}
c,IV/c,III	265.9 K	
c,III/c,II	280.2 K	
c,II/c,I	321.5 K,	ΔH = 4540 J·mol^{-1}
		ΔS = 14.55 J·mol^{-1}·K^{-1}

ΔH and ΔS are total of c,IV/c,III; c,III/c,II; and c,II/c,I transitions.
Molecular Weight 344.0191
Wiswesser Line Notation L6ØJ Ø-FE-- ØL5ØJ &PFFFFFF
Evaluation A

$C_{11}H_{12}O_2$ (liq) 84BEK/RUE
4-Carbomethoxyhomocubane
Heat Capacity 298 K, C_p = 288 J·mol^{-1}·K^{-1}
C_p given as 0.391 cal·K^{-1}·g^{-1}.
Phase Changes

liq/g	303–343 K,	ΔH = 79956 J·mol^{-1}

Derived from vapor pressure measurements.
Molecular Weight 176.2146
Wiswesser Line Notation L444 B4 D5 4ABCD ITJ AVO1
Evaluation B

$C_{11}H_{14}N_2$ (c) 81LEB/RYA
Gramine; 3-Dimethylaminomethyl indole
Heat Capacity C_p = 283.5 J·mol^{-1}·K^{-1}
Temperature range 298 to 393 K.
Data given over temperature range.
Molecular Weight 174.2450
Wiswesser Line Notation T56 BMJ D1N1&1
Evaluation B

$C_{11}H_{16}Si$ (liq) 81LEB/LEB
Vinyldimethylbenzylsilane
Heat Capacity 298.15 K, C_p = 312.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 399.4 J·mol^{-1}·K^{-1}
Phase Changes

c/liq	204.14 K,	ΔH = 11600 J·mol^{-1}
		ΔS = 56.7 J·mol^{-1}·K^{-1}

Molecular Weight 176.3329
Wiswesser Line Notation 1U1-SI-1&1&1R
Evaluation A
T(glass) = 145 K.

$(C_{11}H_{16}Si)_n$ (gls) 81LEB/LEB
Polyvinyldimethylbenzylsilane
Heat Capacity 298.15 K, C_p = 310.5 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Highly elastic state.
Entropy 298.15 K, S = 294.0 J·mol^{-1}·K^{-1}
Highly elastic state.
Molecular Weight 176.3329
Wiswesser Line Notation /*1Y*-SI-1&1&1R/
Evaluation A
T(glass) = 279 K.

$C_{11}H_{17}NO$ (c) 89ABB/JIM
1-Adamantyl carboxamide
Heat Capacity 298.15 K, C_p = 220.5 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.23 J·g^{-1}·K^{-1}.
Phase Changes
c/g 298.15 K, ΔH = 108000 J·mol^{-1}
ΔS = 362.2 J·mol^{-1}·K^{-1}
Molecular Weight 179.2614
Wiswesser Line Notation L66 B6/B-H/DI A B- C 1B ITJ BVZ
Evaluation A

$C_{11}H_{20}$ (c) 75PAR/STE
Bicyclo[3.3.3]undecane; Manxane
Heat Capacity 298.15 K, C_p = 213.2 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/g 298.15 K, ΔH = 6359.7 J·mol^{-1}
ΔS = 21.33 J·mol^{-1}·K^{-1}
Molecular Weight 152.2790
Wiswesser Line Notation T88 A B CTJ
Evaluation B(C_p), A(Phase changes)

$C_{11}H_{20}O_3Si_3$ (liq) 84DZH/KUL
1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane
Heat Capacity 298.15 K, C_p = 519.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 620.8 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 226.84 K, ΔH = 18293 J·mol^{-1}
ΔS = 80.7 J·mol^{-1}·K^{-1}
Molecular Weight 284.5337
Wiswesser Line Notation T6-SI-O-SI-O-SI-OJ A1 A1 C1 C1 E1 ER
Evaluation A
Data given for glassy state from 5 to 226.8 K.
Glass transition at 150 K.

$C_{11}H_{22}O$ (liq) 70HAR/HEA
6-Undecanone
Heat Capacity 298.15 K, C_p = 362.7 J·mol^{-1}·K^{-1}
One temperature. An estimate.
Molecular Weight 170.2942
Wiswesser Line Notation 5V5
Evaluation B

$C_{11}H_{24}O$ (liq) 75FEN/HAR
2-Oxadodecane; Methyl-*n*-decyl ether
Heat Capacity 298.15 K, C_p = 370.5 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 172.3100
Wiswesser Line Notation 10O1
Evaluation B

$C_{12}Cl_{10}$ (c) 87SAI/ATA
Decachlorobiphenyl; Perchlorobiphenyl
Heat Capacity 298.15 K, C_p = 344.0 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 455.8 J·mol^{-1}·K^{-1}
Molecular Weight 498.6620
Wiswesser Line Notation GR BG CG DG EG FR BG CG DG EG FG
Evaluation A

$C_{12}D_{10}$ (c) 87SAI/ATA2
Biphenyl-d_{10}
Heat Capacity 298.15 K, C_p = 228.85 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 230.88 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 20.2 K, ΔH = 0.18 J·mol^{-1}
ΔS = 0.009 J·mol^{-1}·K^{-1}
Lock-in transition.
c,II/c,I 36.8 K, ΔH = 4.61 J·mol^{-1}
ΔS = 0.128 J·mol^{-1}·K^{-1}
Twist transition.
Molecular Weight 164.2900
Wiswesser Line Notation RR &1A-E/H-2 &2A-E/H-2 5
Evaluation A

$C_{12}D_{10}$ (c) 83ATA/SAI
Biphenyl-d_{10}
Heat Capacity
Temperature range 3 to 300 K.
Data given graphically.
Phase Changes
c,III/c,II 20.2 K, ΔH = 0.18 J·mol^{-1}
ΔS = 0.009 J·mol^{-1}·K^{-1}
Anamolous region: 18.5 to 22.5 K.
c,II/c,I 36.8 K, ΔH = 4.61 J·mol^{-1}
ΔS = 0.128 J·mol^{-1}·K^{-1}
Anomalous region: 28 to 44 K.
Molecular Weight 164.2900
Wiswesser Line Notation RR &1A-E/H-2 5 &2A-E/H-2 5
Evaluation A

$C_{12}F_{10}$ (c) 87SAI/ATA
Decafluorobiphenyl; Perfluorobiphenyl
Heat Capacity 298.15 K, C_p = 317.4 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 377.4 J·mol^{-1}·K^{-1}
Molecular Weight 334.1160
Wiswesser Line Notation FR BF CF DF EF FR BF CF DF EF FF
Evaluation A

$C_{12}H_7Cl_2NO_3$ (c) 81VOR/BOR
2,4-Dichloro-4'-nitrodiphenyl ether
Phase Changes
c/liq 343 K, ΔH = 2700 J·mol^{-1}
ΔS = 7.87 J·mol^{-1}·K^{-1}
liq/g 643 K, ΔH = 115900 J·mol^{-1}
ΔS = 180.2 J·mol^{-1}·K^{-1}
Molecular Weight 284.0982
Wiswesser Line Notation WNR DOR BG DG
Evaluation C

$C_{12}H_8Cl_2O_2S$ (c) 85NOV/TSV
4,4'-Dichlorodiphenyl sulphone
Heat Capacity 298.15 K, C_p = 269.3 J·mol^{-1}·K^{-1}
Temperature range 14 to 480 K.
Entropy 298.15 K, S = 314.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 422 K, ΔH = 24400 J·mol^{-1}
ΔS = 57.8 J·mol^{-1}·K^{-1}
Molecular Weight 287.1600
Wiswesser Line Notation GR DSWR DG
Evaluation A

$C_{12}H_8Cl_4Si_2$ (c) 74GEI/DZH
o,o'-Bis-trichlorosilylbiphenyl
Heat Capacity
Temperature range 12 to 370 K.
Deposited in VINITI, No 7671–73, 21 December 1973.
Entropy 298.15 K, $S = 348.4$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 289.5 K, $\Delta H = 57.7$ J·mol^{-1}
$\Delta S = 0.20$ J·mol^{-1}·K^{-1}
trans-cis conformational transition.
c,I/liq 339.18 K, $\Delta H = 20719$ J·mol^{-1}
$\Delta S = 61.09$ J·mol^{-1}·K^{-1}
Molecular Weight 350.1782
Wiswesser Line Notation G-SI-GGR BR B-SI-GGG
Evaluation A

$C_{12}H_8F_2$ (c) 86SAI/ATA
4,4'-Difluorobiphenyl
Heat Capacity 298.15 K, $C_p = 222.77$ J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, $S = 237.59$ J·mol^{-1}·K^{-1}
Phase Changes
liq/g 298.15 K, $\Delta H = 91200$ J·mol^{-1}
$\Delta S = 305$ J·mol^{-1}·K^{-1}
p = 0.5092 Pa, data from 64SMI/GOR.
Molecular Weight 190.1920
Wiswesser Line Notation FR DR DF
Evaluation A

$C_{12}H_8S$ (c) 83ORO/MRA
Dibenzothiophene
Heat Capacity 298.15 K, $C_p = 194.6$ J·mol^{-1}·K^{-1}
Temperature range 220 to 560 K.
$C_p = 0.6709\ (T/\mathrm{K}) - 5.4$ (220 to 371.0 K) J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 371.0 K, $\Delta H = 21580$ J·mol^{-1}
$\Delta S = 58.17$ J·mol^{-1}·K^{-1}
Molecular Weight 184.2552
Wiswesser Line Notation T B656 HSJ
Evaluation A
C_p(liq) = 0.4215 (T/K) + 123.8 (370.1 to 560 K) J·mol^{-1}·K^{-1}.

$C_{12}H_9Cl$ (c) 75GEI/DZH
p-Chlorobiphenyl
Heat Capacity 298.15 K, $C_p = 243.8$ J·mol^{-1}·K^{-1}
Temperature range 12 to 370 K.
Entropy 298.15 K, $S = 256.9$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 348.55 K, $\Delta H = 13318$ J·mol^{-1}
$\Delta S = 38.21$ J·mol^{-1}·K^{-1}
Molecular Weight 188.6561
Wiswesser Line Notation GR DR
Evaluation A
$T/_{\mathrm{Debye}} = 91$ K; see also 77GEI/KAR.

$C_{12}H_9Cl_3Si$ (c) 76GEI/DZH
p-Trichlorosilylbiphenyl
Heat Capacity 298.15 K, $C_p = 291.1$ J·mol^{-1}·K^{-1}
Temperature range 12 to 380 K.
Entropy 298.15 K, $S = 328.8$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I
Anomaly on heat capacity curve from 207 to 221 K.
c/liq 372.90 K, $\Delta H = 18569$ J·mol^{-1}
$\Delta S = 49.80$ J·mol^{-1}·K^{-1}
Molecular Weight 287.6476
Wiswesser Line Notation G-SI-GGR DR
Evaluation A
See also 77GEI/KAR.

$C_{12}H_{10}$ (c) 1889EYK
Biphenyl; Diphenyl
Phase Changes
c/liq 314.3 K, $\Delta H = 18945$ J·mol^{-1}
$\Delta S = 60.3$ J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C

$C_{12}H_{10}$ (c) 79SMI
Biphenyl; Diphenyl
Phase Changes
c/liq 344.1 K, $\Delta H = 18800$ J·mol^{-1}
$\Delta S = 54.6$ J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (c) 82WAS/RAD
Biphenyl; Diphenyl
Heat Capacity 300 K, $C_p = 190$ J·mol^{-1}·K^{-1}
Temperature range 180 to 350 K.
Data given graphically.
Value estimated from graph.
Phase Changes
c,I/liq 343.3 K, $\Delta H = 19900$ J·mol^{-1}
$\Delta S = 58.0$ J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation C(C_p), B(Phase changes)

$C_{12}H_{10}$ (c) 83ATA/SAI
Biphenyl; Diphenyl
Phase Changes
c,III/c,II 16.8 K, $\Delta H = 0.15$ J·mol^{-1}
$\Delta S = 0.009$ J·mol^{-1}·K^{-1}
Anomalous region: 15.3 to 18.3 K.
c,II/c,I 40.4 K, $\Delta H = 5.02$ J·mol^{-1}
$\Delta S = 0.129$ J·mol^{-1}·K^{-1}
Anomalous region: 30 to 47 K.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (c) 83ORO/MRA
Biphenyl; Diphenyl
Heat Capacity 298.15 K, $C_p = 197.7$ J·mol^{-1}·K^{-1}
Temperature range 220 to 475 K.
$C_p = 0.7143\ (T/\mathrm{K}) - 15.3$ (220 to 342.2 K) J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 342.2 K, $\Delta H = 18580$ J·mol^{-1}
$\Delta S = 54.3$ J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A
C_p(liq) = 0.4284 (T/K) + 122.0 (342.2 to 485 K) J·mol^{-1}·K^{-1}.

$C_{12}H_{10}$ (c) 88SAI/ATA
Biphenyl; Diphenyl
Heat Capacity 298.15 K, C_p = 198.17 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 209.00 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 16.8 K, ΔH = 0.15 J·mol^{-1}
ΔS = 0.009 J·mol^{-1}·K^{-1}
Lock-in transition.
c,II/c,I 40.4 K, ΔH = 5.02 J·mol^{-1}
ΔS = 0.129 J·mol^{-1}·K^{-1}
Twist transition.
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation A

$C_{12}H_{10}$ (c) 89CHI/KNI
Biphenyl; Diphenyl
Heat Capacity 298.15 K, C_p = 198.39 mol^{-1}K^{-1}
Temperature Range 5 to 700 K
Entropy 298.15 K, S = 209.38 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 342.098 K, ΔH = 2234.14 J·mol^{-1}
ΔS = 6.5307 J·mol^{-1}·K^{-1}
c/g 298.15 K ΔH = 81520 J·mol^{-1}
ΔS = 273.42 J·mol^{-1}·K^{-1}
Molecular Weight 154.2110
Wiswesser Line Notation RR
Evaluation *A*

$C_{12}H_{10}Cr$ (c) 69AND/WES
Bis(benzene)chromium
Heat Capacity 298.15 K, C_p = 223.93 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Entropy 298.15 K, S = 226.23 J·mol^{-1}·K^{-1}
Molecular Weight 206.2070
Wiswesser Line Notation L6ØJ Ø-CR-- ØL6ØJ
Evaluation A

$C_{12}H_{10}N_2$ (c) 84VAN/BOU
trans-Azobenzene
Heat Capacity 300 K, C_p = 229.3 J·mol^{-1}·K^{-1}
Temperature range 90 to 320 K.
Phase Changes
c/liq 341.03 K, ΔH = 22520 J·mol^{-1}
ΔS = 66.0 J·mol^{-1}·K^{-1}
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR -T
Evaluation B

$C_{12}H_{10}N_2$ (c) 85BOU/DEL
trans-Azobenzene
Heat Capacity 300 K, C_p = 229.33 J·mol^{-1}·K^{-1}
Temperature range 300 to 400 K.
Phase Changes
c,I/liq 341.06 K, ΔH = 22530 J·mol^{-1}
ΔS = 66.06 J·mol^{-1}·K^{-1}
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR -T
Evaluation A

$C_{12}H_{10}N_2$ (c) 1889EYK
Azobenzene
Phase Changes
c/liq 342.2 K, ΔH = 22389 J·mol^{-1}
ΔS = 65.4 J·mol^{-1}·K^{-1}
Molecular Weight 182.2244
Wiswesser Line Notation RNUNR
Evaluation C

$C_{12}H_{10}O_2$ (c) 86SAI/ATA2
p,p'-Biphenol; 4,4'-Dihydroxybiphenyl
Heat Capacity 298.15 K, C_p = 224.31 J·mol^{-1}·K^{-1}
Temperature range 3 to 315 K.
Entropy 298.15 K, S = 220.57 J·mol^{-1}·K^{-1}
Molecular Weight 186.2098
Wiswesser Line Notation QR DR DQ
Evaluation A

$C_{12}H_{12}$ (c,I) 88MES/FIN
2,3-Dimethylnaphthalene
Heat Capacity 298.15 K, C_p = 216.466 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 225.853 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 226.000 K, ΔH = -0.58 J·mol^{-1}
c,II/c,I 265.000 K, ΔH = -1.08 J·mol^{-1}
c,I/liq 377.496 K, ΔH = 19353.29 J·mol^{-1}
ΔS = 51.27 J·mol^{-1}·K^{-1}
Molecular Weight 156.2268
Wiswesser Line Notation L66J C1 D1
Evaluation A

$C_{12}H_{12}CrBr$ (c) 72NIK/SAF
Bis(benzene)chromium bromide
Heat Capacity 298.15 K, C_p = 328.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 339.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 234.6 K
Molecular Weight 288.1268
Wiswesser Line Notation L6ØJ Ø-CR-- ØL6ØJ &E
Evaluation B

$C_{12}H_{12}CrCl$ (c) 72NIK/SAF
Bis(benzene)chromium chloride
Heat Capacity 298.15 K, C_p = 323.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 335.1 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 178.75 K, ΔH = 1820 J·mol^{-1}
ΔS = 10.2 J·mol^{-1}·K^{-1}
Molecular Weight 243.6758
Wiswesser Line Notation L6ØJ Ø-CR-- ØL6ØJ &G
Evaluation B

$C_{12}H_{12}CrI$ (c) 72NIK/SAF
Bis(benzene)chromium iodide
Heat Capacity 298.15 K, C_p = 249.6 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 289.5 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 240.6 K, ΔH = 1695 J·mol^{-1}
ΔS = 7.04 J·mol^{-1}·K^{-1}
Molecular Weight 335.1273
Wiswesser Line Notation L6ØJ Ø-CR-- ØL6ØJ &I
Evaluation B

$C_{12}H_{12}N_2O$ (c) 77KAR/BAZ
4,4'-Diaminodiphenylether
Heat Capacity 300 K, C_p = 258.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, S = 241.0 J·mol^{-1}·K^{-1}
Molecular Weight 200.2396
Wiswesser Line Notation ZR DOR DZ
Evaluation B

$C_{12}H_{12}N_2O$ (c) 87LES/LIC
4,4′-Diaminodiphenyl oxide; 4,4′-Diaminodiphenyl ether
Heat Capacity 298 K, C_p = 278.2 J·mol^{-1}·K^{-1}
Temperature range 250 to 400 K.
Phase Changes
c/liq 464 K
Molecular Weight 200.2396
Wiswesser Line Notation ZR DOR DZ
Evaluation B

$C_{12}H_{12}N_2O_2S$ (c) 87LES/LIC
4,4′-Diaminodiphenyl sulfone
Heat Capacity 298 K, C_p = 314.9 J·mol^{-1}·K^{-1}
Temperature range 250 to 400 K.
Phase Changes
c/liq 451 K
Molecular Weight 248.2990
Wiswesser Line Notation ZR DSWR DZ
Evaluation B

$C_{12}H_{12}N_4O$ (c) 77KAR/RAB
3,3′,4,4′-Tetraaminodiphenyl ether
Heat Capacity 300 K, C_p = 400 J·mol^{-1}·K^{-1}
Temperature range 100 to 700 K.
Data given graphically.
Value estimated from graph.
Entropy 300 K, S = 293.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 402.6 K, ΔH = 25301 J·mol^{-1}
ΔS = 62.8 J·mol^{-1}·K^{-1}
Molecular Weight 228.2532
Wiswesser Line Notation ZR BZ DOR CZ DZ
Evaluation C(C_p),A,(S,Phase changes).

$C_{12}H_{12}O_4$ (c) 89KIR/CHU
1,4-Dimethylcubane dicarboxylate
Heat Capacity 298.15 K, C_p = 251.1 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 437.8 K, ΔH = 41000 J·mol^{-1}
ΔS = 93.7 J·mol^{-1}·K^{-1}
Molecular Weight 220.2250
Wiswesser Line Notation L444 B4 D4 4ABCD HTJ AVO1 HVO1
Evaluation B

$(C_{12}H_{12}O_4)_n$ (gls) 88CHE/PAN
Poly(butylene terephthalate)
Heat Capacity 280 K, C_p = 254 J·mol^{-1}·K^{-1}
Temperature range 210 to 560 K.
Data given graphically.
C_p (J·mol^{-1}·K^{-1}) = 0.000713 T^2 + 0.5203 T + 52.16 (220 to 280 K) for semicrystal.
Phase Changes
c,III/c,II 248 K
Glass transition for amorphous sample.
c,II/c,I 320 K
Glass transition for semicrystalline sample.
c,I/liq 518 K
Molecular Weight 220.2244
Wiswesser Line Notation /*OVR DVO4*/
Evaluation B

$C_{12}H_{15}NO_2$ (liq) 85KAR/ABD2
Phenylaminoethyl methacrylate
Phase Changes
c/liq 297.5 K, ΔH = 25465 J·mol^{-1}
ΔS = 85.60 J·mol^{-1}·K^{-1}
Molecular Weight 205.2560
Wiswesser Line Notation 1UY1&VO2MR
Evaluation A

$C_{12}H_{16}$ (liq) 83ORO/MRA
Cyclohexylbenzene
Heat Capacity 198.15 K, C_p = 263.2 J·mol^{-1}·K^{-1}
Temperature range 220 to 475 K.
C_p(c) = 0.8803 (T/K)− 29.2 (220 to 280.5 K);
C_p(liq) = 0.6130 (T/K) + 80.4 (280.5 to 475 K) J·mol^{-1}·K^{-1}.
Phase Changes
c/liq 280.5 K, ΔH = 15270 J·mol^{-1}
ΔS = 54.44 J·mol^{-1}·K^{-1}
Molecular Weight 160.2584
Wiswesser Line Notation L6TJ AR
Evaluation A

$C_{12}H_{18}$ (c) 82ATA/GYO
Hexamethylbenzene
Heat Capacity 300 K, C_p = 252.11 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 300 K, S = 302.81 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 117.5 K, ΔH = 990 J·mol^{-1}
ΔS = 8.3 J·mol^{-1}·K^{-1}
First order transition.
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A
An additional thermal anomaly producing a hump in the heat capacity curve with a maximum of 50 J·mol^{-1}·K^{-1} at 128 K is hidden behind the first order transition.

$C_{12}H_{18}$ (c) 85YOS/FUJ
Hexamethylbenzene
Phase Changes
c,II/c,I 115.5 K, ΔH = 1103 J·mol^{-1}
ΔS = 9.55 J·mol^{-1}·K^{-1}
Molecular Weight 162.2742
Wiswesser Line Notation 1R B1 C1 D1 E1 F1
Evaluation A

$C_{12}H_{18}Be_4O_{13}$ (c) 47JAF
Beryllium oxyacetate
Heat Capacity 298.95 K, C_p = 553.1 J·mol^{-1}·K^{-1}
Temperature range 297 to 332 K.
Unsmoothed experimental datum.
Molecular Weight 406.3151
Wiswesser Line Notation OV1 6 .BE 4 &O
Evaluation C

$C_{12}H_{18}Be_4O_{13}$ (c) 55MOM/SEK
Beryllium oxyacetate
Heat Capacity 298.85 K, C_p = 514.6 J·mol^{-1}·K^{-1}
Temperature range 273 to 370 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 315 K
Lambda type transition at 315 K.
Transitions also indicated at 305, 350 and 398 K.
c,I/liq 421 K, ΔH = 27196 J·mol^{-1}
ΔS = 48.5 J·mol^{-1}·K^{-1}
Molecular Weight 406.3151
Wiswesser Line Notation OV1 6 .BE 4 &O
Evaluation B(C_p), A(Phase changes)

$C_{12}H_{18}O_2$ (liq) 77KAR/SAP
Acetophenone diethyl ketal
Heat Capacity 298 K, C_p = 210 J·mol^{-1}·K^{-1}
Temperature range 60 to 340 K.
C_p data calculated from equation:
$C_p = (475)(0.71198 - 0.000908T)$.
Molecular Weight 194.2730
Wiswesser Line Notation 2OX1&O2&R
Evaluation D

$C_{12}H_{18}O_2$ (gls) 78KAR/SAP
Acetophenone diethyl ketal
Entropy 298.15 K, S = 364.3 J·mol^{-1}·K^{-1}
Molecular Weight 194.2730
Wiswesser Line Notation 2OX1&O2&R
Evaluation A
T(glass) = 173.2 K.

$C_{12}H_{20}O_6$ (liq) 86NIL/WAD
Tripropionin
Heat Capacity 298.15 K, C_p = 481.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 260.2864
Wiswesser Line Notation 2VO1YOV2&1OV2
Evaluation A

$C_{12}H_{22}$ (liq) 83ORO/MRA
Bicyclohexyl
Heat Capacity 298.15 K, C_p = 283.0 J·mol^{-1}·K^{-1}
Temperature range 220 to 475 K.
C_p = 0.7589 (T/K) + 56.7 (277.2 to 475 K) J·mol^{-1}·K^{-1}.
Phase Changes
c,IV/c,III 256.1 K, ΔH = 1540 J·mol^{-1}
c,III/c,II 267.5 K, ΔH = 740 J·mol^{-1}
c,II/c,I 273.5 K, ΔH = 7080 J·mol^{-1}
c,I/liq 277.2 K, ΔH = 6780 J·mol^{-1}
Molecular Weight 166.3058
Wiswesser Line Notation L6TJ A- AL6TJ
Evaluation A

$C_{12}H_{22}O_2$ (liq) 85KAR/ABD
Octyl methacrylate
Heat Capacity 298.15 K, C_p = 386.0 J·mol^{-1}·K^{-1}
Temperature range 230 to 350 K.
C_p (J·kg^{-1}·K^{-1}) = 1261.8 + 2.2971 T.
C_p data calculated from equation.
Phase Changes
c/liq 230.3 K
Molecular Weight 198.3046
Wiswesser Line Notation 8OVY1&U1
Evaluation B

$C_{12}H_{22}O_2$ (liq) 85KAR/ABD2
Octyl methacrylate
Phase Changes
c/liq 230.3 K, ΔH = 24085 J·mol^{-1}
ΔS = 104.6 J·mol^{-1}·K^{-1}
Molecular Weight 198.3046
Wiswesser Line Notation 8OVY1&U1
Evaluation A

$C_{12}H_{22}O_2$ (liq) 85KAR/ABD2
Nonyl acrylate
Phase Changes
c/liq 236.5 K, ΔH = 23362 J·mol^{-1}
ΔS = 98.8 J·mol^{-1}·K^{-1}
Molecular Weight 198.3046
Wiswesser Line Notation 9OV1U1
Evaluation A

$C_{12}H_{22}O_6$ (liq) 82BAB/RAB
Oligoethylene butylene glycol adipate;
1,4-Butylene glycol-ethylene glycol-adipic acid oligomer
Heat Capacity 298.15 K, C_p = 482.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
C_p = 1.839 kJ·kg^{-1}·K^{-1} at 298.15 K.
Entropy 298.15 K, S = 471.1 J·mol^{-1}·K^{-1}
S° = 1.796 kJ·kg^{-1}·K^{-1} at 298.15 K.
Phase Changes
gls/liq 207 K ΔH = 11565 J·mol^{-1}
ΔS = 55.87 J·mol^{-1}·K^{-1}
Molecular Weight 262.3022
Wiswesser Line Notation Q4OV4VO2Q
Evaluation A
Data for glassy oligomer to liquid oligomer.

$C_{12}H_{22}O_6$ (liq) 82BAB/RAB
Oligoethylene butylene glycol adipate;
1,4-Butylene glycol-ethylene glycol-adipic acid oligomer
Heat Capacity 298.15 K, C_p = 482.4 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
C_p = 1.839 kJ·kg^{-1}·K^{-1} at 298.15 K.
Entropy 298.15 K, S = 527.0 J·mol^{-1}·K^{-1}
S° = 2.009 kJ·kg^{-1}·K^{-1} at 298.15 K.
Phase Changes
c,I/liq 290.7 K, ΔH = 32709 J·mol^{-1}
ΔS = 112.5 J·mol^{-1}·K^{-1}
Molecular Weight 262.3022
Wiswesser Line Notation Q4OV4VO2Q
Evaluation A
Data for crystalline oligomer to liquid oligomer.

$C_{12}H_{22}O_{11}$ (c) 03MAG
Sucrose; Cane sugar
Heat Capacity 298 K, C_p = 431.1 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.301 cal·g^{-1}·K^{-1}.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ B1Q CQ DQ EQ FO-BT5OTJ B1Q CQ DQ E1Q—A&BD -B&CEF—A&BD -B&CE
Evaluation D

$C_{12}H_{22}O_{11}$ (c) 03MAG
Maltose
Heat Capacity 298 K, C_p = 461.2 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.322 cal·g^{-1}·K^{-1}.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO-BT6OTJ CQ DQ EQ F1Q—A&CE -B&BDF—A&BCE—B&DF
Evaluation D

$C_{12}H_{22}O_{11}$ (c) 03MAG
Lactose, anhydrous; Milk sugar
Heat Capacity 298 K, C_p = 412.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.288 cal·g^{-1}·K^{-1}.
Molecular Weight 342.2992
Wiswesser Line Notation T6OTJ BQ CQ DQ F1Q EO-BT6OTJ CQ DQ EQ F1Q—A&CE -B&BDF—A&C—B&BDEF
Evaluation D

$C_{12}H_{23}O_2Tl$ (c) 76MEI/SEY
Thallium *n*-dodecanoate
Phase Changes
c,III/c,II 312 K, ΔH = 3807 J·mol^{-1}
ΔS = 12.1 J·mol^{-1}·K^{-1}
c,II/c,I 354 K, ΔH = 2427 J·mol^{-1}
ΔS = 6.69 J·mol^{-1}·K^{-1}
liq/liq 471 K, ΔH = 1925 J·mol^{-1}
ΔS = 4.10 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,I/liq 398 K, ΔH = 5858 J·mol^{-1}
ΔS = 14.2 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 403.6825
Wiswesser Line Notation OV11 .TL
Evaluation B

$C_{12}H_{23}O_2Tl$ (c) 87LOP/WES
Thallium *n*-dodecanoate
Heat Capacity 298.15 K, C_p = 471.84 J·mol^{-1}·K^{-1}
Temperature range 7 to 470 K.
Entropy 298.15 K, S = 451.06 J·mol^{-1}·K^{-1}
Phase Changes
c,VI/c,V 283.0 K, ΔH = 1829 J·mol^{-1}
ΔS = 6.49 J·mol^{-1}·K^{-1}
c,V/c,IV 285.2 K, ΔH = 2087 J·mol^{-1}
ΔS = 7.32 J·mol^{-1}·K^{-1}
c,IV/c,III 293.6 K, ΔH = 1413 J·mol^{-1}
ΔS = 4.82 J·mol^{-1}·K^{-1}
c,III/c,II 312.3 K, ΔH = 4490 J·mol^{-1}
ΔS = 14.38 J·mol^{-1}·K^{-1}
c,II/c,I 356.6 K, ΔH = 2054 J·mol^{-1}
ΔS = 5.74 J·mol^{-1}·K^{-1}
c,I/liq 400.1 K, ΔH = 5454 J·mol^{-1}
ΔS = 13.64 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 471.6 K, ΔH = 1971 J·mol^{-1}
ΔS = 4.16 J·mol^{-1}·K^{-1}
Mesophase-isotropic liquid.
Molecular Weight 403.6825
Wiswesser Line Notation OV11 .TL
Evaluation A

$C_{12}H_{24}O_2$ (c) 86KAL/JAC
Butyl octadecanoate
Phase Changes
c,II/c,I 288.4 K, ΔH = 2220 J·mol^{-1}
ΔS = 7.70 J·mol^{-1}·K^{-1}
c,I/liq 299.72 K, ΔH = 37480 J·mol^{-1}
ΔS = 121.5 J·mol^{-1}·K^{-1}
Molecular Weight 200.3204
Wiswesser Line Notation 7VO4
Evaluation A

$C_{12}H_{26}$ (liq) 81GRO/ING
n-Dodecane
Heat Capacity 298.15 K, C_p = 374.82 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 82ZAR
n-Dodecane
Heat Capacity 298 K, C_p = 374.5 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 84GRO/BEN
n-Dodecane
Heat Capacity 298.15 K, C_p = 375.26 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 84KUM/BEN
n-Dodecane
Heat Capacity 298.15 K, C_p = 375.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 84ROU/GRO
n-Dodecane
Heat Capacity 298.15 K, C_p = 374.93 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 86TAR/AIC
n-Dodecane
Heat Capacity 298.15 K, C_p = 376.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 86WIL/LAI
n-Dodecane
Heat Capacity 298.15 K, C_p = 373.30 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 88COS/HUU
n-Dodecane
Heat Capacity 298.15 K, C_p = 376.09 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation B

$C_{12}H_{26}$ (liq) 88PER/AIC
n-Dodecane
Heat Capacity 298.15 K, C_p = 376.00 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 12H
Evaluation A

$C_{12}H_{26}$ (liq) 88COS/HUU
2,2,4,6,6-Pentamethylheptane
Heat Capacity 298.15 K, C_p = 350.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 1X1&1&1Y1&1X1&1&1
Evaluation B

$C_{12}H_{26}$ (liq) 88PER/AIC
2,2,4,6,6-Pentamethylheptane
Heat Capacity 298.15 K, C_p = 350.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 170.3374
Wiswesser Line Notation 1X1&1&1Y1&1X1&1&1
Evaluation A

$C_{12}H_{26}O_5$ (liq) 82ZAR
Tetrapropylene glycol
Heat Capacity 298 K, C_p = 560.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 250.3344
Wiswesser Line Notation QYOYOYOYQ
Evaluation B

$C_{12}H_{26}O_7$ (liq) 82ZAR
Hexaethylene glycol
Heat Capacity 298 K, C_p = 620.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 282.3332
Wiswesser Line Notation Q2O2O2O2O2O2Q
Evaluation B

$C_{12}H_{27}O_4P$ (liq) 81NAZ/RUD
Tri-*n*-butylphosphate
Heat Capacity 298.15 K, C_p = 379.4 J·mol^{-1}·K^{-1}
Temperature range 283 to 423 K.
C_p given as 1.404 J·g^{-1}·K^{-1} at 20 °C and 1.445 J·g^{-1}·K^{-1} at 30 °C.
Molecular Weight 266.3167
Wiswesser Line Notation OPO4&O4&O4
Evaluation B

$C_{12}H_{28}ClN$ (c) 88VAN/WHI
Di-*n*-hexylammonium chloride
Heat Capacity 300.92 K, C_p = 408.6 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K.
Unsmoothed experimental datum.
Phase Changes
c,III/c,II 115.25 K, ΔH = 908 J·mol^{-1}
ΔS = 7.89 J·mol^{-1}·K^{-1}
c,II/c,I 279.39 K, ΔH = 15950 J·mol^{-1}
ΔS = 57.38 J·mol^{-1}·K^{-1}
Molecular Weight 221.8129
Wiswesser Line Notation 6M6 &GH
Evaluation A

$C_{12}H_{28}S$ (liq) 82TUT/GAB
1-Dodecanethiol; *n*-Dodecyl mercaptan
Heat Capacity 300 K, C_p = 442.81 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 423.01 + 3.878\times10^{-2}\,T + 9.070\times10^{-5}\,T^2$.
Molecular Weight 204.4132
Wiswesser Line Notation SH12
Evaluation B

$C_{12}H_{30}O_3Si_3$ (liq) 82KUL/LEB
1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p = 535.3 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S = 674.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 140–160 K, ΔH = 470 J·mol^{-1}
Glassy transition.
c,II/c,I 242.3 K, ΔH = 11730 J·mol^{-1}
ΔS = 48.41 J·mol^{-1}·K^{-1}
c,I/liq 283.41 K, ΔH = 11940 J·mol^{-1}
Molecular Weight 306.6237 ΔS = 42.1 J·mol^{-1}·K^{-1}
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2
Evaluation A

$C_{12}H_{30}O_3Si_3$ (liq) 84LEB/KUL
1,1,3,3,5,5,-Hexaethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p = 535.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Entropy 298.15 K, S = 671.4 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 140–168 K, ΔH = 470 J·mol^{-1}
Glassy transition.
c,II/c,I 242.3 K, ΔH = 11700 J·mol^{-1}
ΔS = 48.4 J·mol^{-1}·K^{-1}
c,I/liq 283.24 K, ΔH = 11940 J·mol^{-1}
ΔS = 42.2 J·mol^{-1}·K^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2
Evaluation A

$C_{12}H_{30}O_3Si_3$ (liq) 85DZH/KUL
1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Heat Capacity 298.15 K, C_p = 581.4 J·mol^{-1}·K^{-1}
Temperature range 5 to300 K.
Entropy 298.15 K, S = 680.8 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 160 K, ΔH = 462 J·mol^{-1}
ΔS = 2.9 J·mol^{-1}·K^{-1}
c,II/c,I 242.3 K, ΔH = 11824 J·mol^{-1}
ΔS = 48.8 J·mol^{-1}·K^{-1}
c,I/liq 280.2 K, ΔH = 11424 J·mol^{-1}
ΔS = 40.9 J·mol^{-1}·K^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2

$C_{12}H_{30}O_3Si_3$ (liq) 88LEB/KUL
1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Heat Capacity 300 K, C_p = 536.53 J·mol^{-1}·K^{-1}
Temperature range 13.4 to 350 K.
Entropy 300 K, S = 674.71 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 140–168 K, ΔH = 470.0 J·mol^{-1}
ΔS = 2.08 J·mol^{-1}·K^{-1}
c,II/c,I 242.4 K, ΔH = 11730.8 J·mol^{-1}
ΔS = 48.39 J·mol^{-1}·K^{-1}
c,I/liq 283.41 K, ΔH = 11940.3 J·mol^{-1}
ΔS = 42.07 J·mol^{-1}·K^{-1}
Molecular Weight 306.6237
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2
Evaluation A

$C_{12}H_{52}Cr_4N_{12}O_{18}S_3 \cdot 10H_2O$ (c) 72MOR/SEK
Hexahydroxyhexaethylenediamine chromium sulfate decahydrate
Heat Capacity 197.459 K, C_p = 1001.82 J·mol^{-1}·K^{-1}
Temperature range 1.4 to 200 K.
Unsmoothed experimental datum.
Molecular Weight 1136.9284
Wiswesser Line Notation CR 4 &Q 6 &Z2Z 6 &S-O4*3 &QH 1O
Evaluation A

$C_{13}H_8Cl_2O$ (c) 87ECO/BER
p-Dichlorobenzophenone
Heat Capacity
Temperature range 175 to 205 K.
Data given graphically.
Phase Changes
c,III/c,II 186.1 K, ΔH = 146 J·mol^{-1}
c,II/c,I 189.5 K, ΔH = 251 J·mol^{-1}
Molecular Weight 251.1116
Wiswesser Line Notation GR DVR DG
Evaluation B

$C_{13}H_9N$ (c) 88STE/CHI
7,8-Benzoquinoline
Heat Capacity 298.15 K, C_p = 206.36 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 213.20 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 324.104 K, ΔH = 14103 J·mol^{-1}
ΔS = 43.51 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T B666 CNJ
Evaluation A

$C_{13}H_9N$ (c) 89STE/CHI
7,8-Benzoquinoline
Heat Capacity 298.15 K, C_p = 206.36 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 213.20 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 324.104 K, ΔH = 14103 J·mol^{-1}
ΔS = 43.51 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T B666 CNJ
Evaluation A

$C_{13}H_9N$ (c) 86STE/CHI
Phenanthridine
Heat Capacity 298.15 K, C_p = 201.79 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, S = 205.87 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 354.16 K
c,I/liq 379.742 K
Molecular Weight 179.2208
Wiswesser Line Notation T B666 HNJ
Evaluation A

$C_{13}H_9N$ (c) 88STE/CHI
Phenanthridine
Heat Capacity 298.15 K, C_p = 201.87 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 205.91 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 354.0 K, ΔH = 20.79 J·mol^{-1}
ΔS = 0.059 J·mol^{-1}·K^{-1}
Extrapolated value.
c,I/liq 379.74 K, ΔH = 22831 J·mol^{-1}
ΔS = 60.12 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T B666 HNJ
Evaluation A

$C_{13}H_9N$ (c) 89STE/CHI
Phenanthridine
Heat Capacity 298.15 K, C_p = 201.87 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 205.91 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 354.0 K, ΔH = 20.79 J·mol^{-1}
ΔS = 0.059 J·mol^{-1}·K^{-1}
Extrapolated value.
c,I/liq 379.74 K, ΔH = 22831 J·mol^{-1}
ΔS = 60.12 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T B666 HNJ
Evaluation A

$C_{13}H_9N$ (c) 86STE/CHI
Acridine
Heat Capacity 298.15 K, C_p = 204.98 J·mol^{-1}·K^{-1}
Temperature range 6 to 450 K.
Entropy 298.15 K, S = 208.00 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.243 K
Molecular Weight 179.2208
Wiswesser Line Notation T C666 BNJ
Evaluation A

$C_{13}H_9N$ (c) 88STE/CHI
Acridine
Heat Capacity 298.15 K, C_p = 205.07 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 208.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.242 K, ΔH = 20682 J·mol^{-1}
ΔS = 53.97 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T C666 BNJ
Evaluation A

$C_{13}H_9N$ (c) 89STE/CHI
Acridine
Heat Capacity 298.15 K, C_p = 205.07 J·mol^{-1}·K^{-1}
Temperature range 5 to 500 K.
Entropy 298.15 K, S = 208.03 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 383.242 K, ΔH = 20682 J·mol^{-1}
ΔS = 53.97 J·mol^{-1}·K^{-1}
Molecular Weight 179.2208
Wiswesser Line Notation T C666 BNJ
Evaluation A

$C_{13}H_{10}N_2$ (liq) 84LEB/BYK
Diphenylcarbodiimide
Heat Capacity 298.15 K, C_p = 304.6 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 330 K.
Entropy 298.15 K, S = 330.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 287.41 K, ΔH = 18550 J·mol^{-1}
ΔS = 64.54 J·mol^{-1}·K^{-1}
Molecular Weight 194.2354
Wiswesser Line Notation RNUCUNR
Evaluation A
Data also given for the vitreous state and supercooled liquid from 5 to 287.41 K.
T(glass) = 190 ± 1 K.

$C_{13}H_{10}O$ (c) 1889EYK
Benzophenone
Phase Changes
c/liq 321.2 K, ΔH = 17669 J·mol^{-1}
ΔS = 55.0 J·mol^{-1}·K^{-1}
Molecular Weight 182.2214
Wiswesser Line Notation RVR
Evaluation C

$C_{13}H_{10}O$ (c) 83DEK/VAN
Benzophenone
Heat Capacity 300 K, C_p = 224.80 J·mol^{-1}·K^{-1}
Temperature range 80 to345 K.
Phase Changes
c/liq 321.03 K, ΔH = 18194 J·mol^{-1}
ΔS = 56.67 J·mol^{-1}·K^{-1}
Molecular Weight 182.2214
Wiswesser Line Notation RVR
Evaluation A
C_p(c) = 40.42 + 0.4252 (T/K) + 6.27021×10^{-4} (T/K)^2 (80 to 290 K) J·mol^{-1}·K^{-1}.
C_p(liq) = 150.19 + 0.4576 (T/K) (280 to 350 K) J·mol^{-1}.

$C_{13}H_{11}N$ (c) 86STE/CHI
N-Methylcarbazole
Heat Capacity 298.15 K, C_p = 217.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 234.30 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 362.490 K
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}N$ (c) 87MES/TOD
N-Methylcarbazole
Heat Capacity 298.15 K, C_p = 217.84 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 234.30 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 362.490 K, ΔH = 17153.8 J·mol^{-1}
ΔS = 47.32 J·mol^{-1}·K^{-1}
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{11}N$ (c) 88MES/TOD
N-Methylcarbazole
Heat Capacity 298.150 K, C_p = 217.838 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.150 K, S = 234.300 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 362.490 K, ΔH = 17153.71 J·mol^{-1}
ΔS = 47.32 J·mol^{-1}·K^{-1}
Molecular Weight 181.2366
Wiswesser Line Notation T B656 HNJ H1
Evaluation A

$C_{13}H_{12}$ (c) 1889EYK
Diphenylmethane
Phase Changes
c/liq 299.4 K, ΔH = 19050 J·mol^{-1}
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation C

$C_{13}H_{12}$ (c) 86CHI/ANN
Diphenylmethane
Phase Changes
c/liq ΔH = 19246 J·mol^{-1}
c/g ΔH = 83262 J·mol^{-1}
Molecular Weight 168.2378
Wiswesser Line Notation R1R
Evaluation A

$C_{13}H_{12}D_{10}FeN_6S_3$ (c) 86SOR/SHI
Ferrocene-d_{10} thiourea clathrate (1:3)
Heat Capacity 300 K, C_p = 510 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Data given graphically.
Value given is an estimate from graph.
Phase Changes
c,VI/c,V 145.8 K, ΔH = 57 J·mol^{-1}
ΔS = 0.39 J·mol^{-1}·K^{-1}
c,V/c,IV 160.6 K, ΔH = 1762 J·mol^{-1}
ΔS = 10.62 J·mol^{-1}·K^{-1}
c,IV/c,III 173.4 K, ΔH = 11 J·mol^{-1}
ΔS = 0.07 J·mol^{-1}·K^{-1}
c,III/c,II 187.1 K, ΔH = 31 J·mol^{-1}
ΔS = 0.17 J·mol^{-1}·K^{-1}
c,II/c,I 219.0 K, ΔH = 57 J·mol^{-1}
ΔS = 0.27 J·mol^{-1}·K^{-1}
Molecular Weight 424.4630
Wiswesser Line Notation L5ØJ Ø-FE-- ØL5ØJ &ZYZUS 3 &1/H-2 5 &14/H-2 5
Evaluation A

$C_{13}H_{12}N_2O$ (c) 87FER/DEL
1,3-Diphenylurea
Phase Changes
c/liq 512.1 K, ΔH = 34620 J·mol^{-1}
ΔS = 66.5 J·mol^{-1}·K^{-1}
Molecular Weight 212.2506
Wiswesser Line Notation RNVNR
Evaluation A

$C_{13}H_{14}N_2$ (c) 87LES/LIC
Bis(4-aminophenyl)methane
Heat Capacity 298 K, C_p = 270.9 J·mol^{-1}·K^{-1}
Temperature range 250 to 400 K.
Phase Changes
c/liq 366 K
Molecular Weight 198.2670
Wiswesser Line Notation ZR D1R DZ
Evaluation B

$C_{13}H_{14}N_2O_2$ (c) 86KAR/BAB
3,3′-Methylene bis(6-aminophenol)
Heat Capacity 298.15 K, C_p = 281.2 J·mol^{-1}·K^{-1}
Temperature range 5 to 470 K.
Entropy 298.15 K, S = 284.6 J·mol^{-1}·K^{-1}
Molecular Weight 230.2658
Wiswesser Line Notation ZR BQ D1R CQ DZ
Evaluation A

$C_{13}H_{15}NO$ (liq) 86ACH/HAS
1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene
Heat Capacity 333 K, C_p = 382 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K.
C_p = 1.9 J·g^{-1}·C^{-1}.
Molecular Weight 201.2676
Wiswesser Line Notation OCNX2&1&R CYU1&1
Evaluation C
98% purity.

$C_{13}H_{15}NO$ (liq) 86ACH/HAS
1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene
Heat Capacity 333 K, C_p = 362 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K.
C_p = 1.8 J·g^{-1}·C^{-1}.
Molecular Weight 201.2676
Wiswesser Line Notation OCNX2&1&R DYU1&1
Evaluation C
91% purity.

$C_{13}H_{20}O$ (liq) 88BAG/GUR
6,10-Dimethyl-4,5,9-undecatrien-2-one
Heat Capacity 313.65 K, C_p = 413.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 192.3004
Wiswesser Line Notation 1YU3YU1U2V1
Evaluation B

$C_{13}H_{20}O$ (liq) 88BAG/GUR
6,10-Dimethyl-3,5,9-undecatrien-2-one
Heat Capacity 297.85 K, C_p = 382.7 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 192.3004
Wiswesser Line Notation 1YU3YU2U1V1
Evaluation B

$C_{13}H_{20}O$ (liq) 88BAG/GUR
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
Heat Capacity 313.60 K, C_p = 388.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 192.3004
Wiswesser Line Notation L6 AUTJ A1 B1U1V1C1 C1
Evaluation B

$C_{13}H_2O_8$ (liq) 83SAN/CIO
Diethylene glycol-glycerol-adipate polymer
Heat Capacity 298.15 K, C_p = 1287 J·mol^{-1}·K^{-1}
Temperature range 273.15 to 323.15 K.
C_p°(kJ kg^{-1}K^{-1}) = 0.023598T - 2.835
Molecular Weight 306.3120
Wiswesser Line Notation /*O2O2OV4VO1YQ71O*/
Evaluation D
Authors did not provide formula for repeating unit of polymer; assumed: glycol-adipate-glycerol, as repeating unit.

$C_{13}H_{24}O_2$ (c) 81LEB/EVS
Tridecanolactone
Heat Capacity 298.15 K, C_p = 398.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S = 401.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 290.63 K, ΔH = 18150 J·mol^{-1}
ΔS = 62.45 J·mol^{-1}·K^{-1}
c,I/liq 300.4 K, ΔH = 9060 J·mol^{-1}
ΔS = 30.2 J·mol^{-1}·K^{-1}
Molecular Weight 212.3314
Wiswesser Line Notation T-14-VOTJ
Evaluation A

$(C_{13}H_{24}O_2)_n$ (c) 81LEB/EVS
Poly(tridecanolactone)
Heat Capacity 298.15 K, C_p = 329.3 J·mol^{-1}·K^{-1}
Temperature range 5 to 400 K.
Entropy 298.15 K, S = 351.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 229 K
Glass/crystal.
c/liq 368.1 K, ΔH = 46000 J·mol^{-1}
ΔS = 125 J·mol^{-1}·K^{-1}
Molecular Weight 212.3314
Wiswesser Line Notation /*OV-14-*/
Evaluation A

$C_{13}H_{26}O$ (liq) 88BAG/GUR
6,10-Dimethyl-2-undecanone
Heat Capacity 313.55 K, C_p = 428.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 198.3478
Wiswesser Line Notation 1Y3Y3V1
Evaluation B

$C_{13}H_{28}O$ (c) 83MAS/STE
tri-*tert*-Butylmethanol
Heat Capacity 298.15 K, C_p = 350.6 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 1.75 J·g^{-1}·K^{-1}
Phase Changes
c,II/c,I 302.17 K, ΔH = 7200 J·mol^{-1}
ΔS = 24 J·mol^{-1}·K^{-1}
Solid-plastic.
c/liq 390.15 K, ΔH = 3430 J·mol^{-1}
ΔS = 8.8 J·mol^{-1}·K^{-1}
Molecular Weight 200.3636
Wiswesser Line Notation QXX1&1&1&X1&1&1&X1&1&1
Evaluation B

$C_{14}H_9NO_2$ (c) 77KAR/BAZ
Phthalanilic acid
Heat Capacity 300 K, C_p = 279.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, S = 322.9 J·mol^{-1}·K^{-1}
Molecular Weight 223.2306
Wiswesser Line Notation QVR BVMR
Evaluation B

$C_{14}H_{10}$ (c) 87RAI/SIN
Phenanthrene
Phase Changes
c/liq (373) K, ΔH = 18627 J·mol^{-1}
ΔS = 49.9 J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation B

$C_{14}H_{10}$ (c) 88TOR/BAR
Phenanthrene
Phase Changes
liq/g 350 K, $\Delta H = 87240$ J·mol^{-1}
$\Delta S = 249.3$ J·mol^{-1}·K^{-1}
c/g 298.15 K, $\Delta H = 90900$ J·mol^{-1}.
$\Delta S = 304.9$ J·mol^{-1}·K^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation L B666J
Evaluation A

$C_{14}H_{10}$ (c) 86CHI/ANN
Diphenylacetylene; Diphenylethyne
Phase Changes
c/liq $\Delta H = 20502$ J·mol^{-1}
c/g $\Delta H = 90374$ J·mol^{-1}
Molecular Weight 178.2330
Wiswesser Line Notation R1UU1R
Evaluation A

$C_{14}H_{10}O_2$ (c) 72BOO/HAU
Benzil; Diphenyl diketone
Phase Changes
c/liq 368.05 K, $\Delta H = 22690$ J·mol^{-1}
$\Delta S = 61.65$ J·mol^{-1}·K^{-1}
Molecular Weight 210.2318
Wiswesser Line Notation RVVR
Evaluation C

$C_{14}H_{10}O_2$ (c) 83DWO
Benzil; Diphenyl diketone
Heat Capacity 298.15 K, $C_p = 245.7$ J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, $S = 292.08$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 84.07 K, $\Delta H = 44.1$ J·mol^{-1}
$\Delta S = 0.52$ J·mol^{-1}·K^{-1}
Molecular Weight 210.2318
Wiswesser Line Notation RVVR
Evaluation A

$C_{14}H_{11}NO_3$ (c) 77KAR/BAZ
N-Phenylphthalimide
Heat Capacity 300 K, $C_p = 245.9$ J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, $S = 273.0$ J·mol^{-1}·K^{-1}
Molecular Weight 241.2458
Wiswesser Line Notation T56 BVNVJ CR
Evaluation B

$C_{14}H_{12}$ (c) 87CHI/HOS
9,10-Dihydrophenanthrene
Heat Capacity 298.15 K, $C_p = 243.08$ J·mol^{-1}·K^{-1}
Temperature range 10 to 350 K.
Entropy 298.15 K, $S = 229.29$ J·mol^{-1}·K^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation L B666&T&J
Evaluation A
Heat capacity and entropy data given for liquid state at 298.15 K:
$C_p = 278.04$,
S° = 270.14 J·mol^{-1}·K^{-1}.

$C_{14}H_{12}$ (c) 87CHI/HOS2
9,10-Dihydroanthracene
Heat Capacity 298.15 K, $C_p = 219.06$ J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Entropy 298.15 K, $S = 218.97$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 382.18 K, $\Delta H = 23840$ J·mol^{-1}
$\Delta S = 62.38$ J·mol^{-1}·K^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation L C666&T&J
Evaluation A

$C_{14}H_{12}$ (c) 84VAN/BOU
trans-Stilbene
Heat Capacity 298.15 K, $C_p = 235.0$ J·mol^{-1}·K^{-1}
Temperature range 8 to 350 K.
Entropy 298.15 K, $S = 247.0$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 398 K, $\Delta H = 27370$ J·mol^{-1}
$\Delta S = 68.8$ J·mol^{-1}·K^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R -T
Evaluation B

$C_{14}H_{12}$ (c) 85BOU/DEL
trans-Stilbene
Heat Capacity 320 K, $C_p = 251.08$ J·mol^{-1}·K^{-1}
Temperature range 320 to 410 K.
Phase Changes
c,I/liq 397.40 K, $\Delta H = 27690$ J·mol^{-1}
$\Delta S = 69.6$ J·mol^{-1}·K^{-1}
Molecular Weight 180.2488
Wiswesser Line Notation R1U1R -T
Evaluation A

$(C_{14}H_{12}Ge)n$ (gls) 78LEB/RAB
Polyvinylenediphenylgermyl-α,ω-dihydride
Heat Capacity 298.15 K, $C_p = 334.7$ J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, $S = 323.2$ J·mol^{-1}·K^{-1}
Highly elastic state.
Molecular Weight 252.8588
Wiswesser Line Notation /*-GE-R&R&1U1*/
Evaluation A
T(glass) = 237 K.

$(C_{14}H_{12}Si)_n$ (gls) 78LEB/RAB
Polyvinylenediphenylsilyl-α,ω-dihydride
Heat Capacity 298.15 K, $C_p = 331.2$ J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, $S = 298.0$ J·mol^{-1}·K^{-1}
Highly elastic state.
Molecular Weight 208.3343
Wiswesser Line Notation /*-SI-R&R&1U1*/
Evaluation A
T(glass) = 264 K.

$C_{14}H_{14}$ (liq) 87CHI/HOS2
Phenyl-o-tolylmethane
Heat Capacity 298.15 K, $C_p = 296.58$ J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Entropy 298.15 K, $S = 335.50$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 279.76 K, $\Delta H = 19241$ J·mol^{-1}
$\Delta S = 68.78$ J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation 1R B1R
Evaluation A

$C_{14}H_{14}$ (liq) 87CHI/HOS
2,2′-Dimethylbiphenyl
Heat Capacity 298.15 K, C_p = 298.06 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 332.60 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 293.091 K, ΔH = 2279.9 J·mol^{-1}
ΔS = 7.78 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation 1R BR B1
Evaluation A

$C_{14}H_{14}$ (liq) 87CHI/HOS
2-Ethylbiphenyl
Heat Capacity 298.15 K, C_p = 302.73 J·mol^{-1}·K^{-1}
Temperature range 5 to 440 K.
Entropy 298.15 K, S = 332.69 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 267.076 K, ΔH = 2068.0 J·mol^{-1}
ΔS = 7.74 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation 2R BR
Evaluation A

$C_{14}H_{14}$ (liq) 87CHI/HOS
1,2,3,4-Tetrahydrophenanthrene
Heat Capacity 298.15 K, C_p = 278.26 J·mol^{-1}·K^{-1}
Temperature range 5 to 430 K.
Entropy 298.15 K, S = 286.60 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 282.5 K, ΔH = 213 J·mol^{-1}
ΔS = 0.75 J·mol^{-1}·K^{-1}
c,II/c,I 298.0 K, ΔH = 1344.2 J·mol^{-1}
ΔS = 4.44 J·mol^{-1}·K^{-1}
c,I/liq 302.560 K
Molecular Weight 182.2646
Wiswesser Line Notation L B666T&&J
Evaluation A

$C_{14}H_{14}$ (c,II) 87CHI/HOS2
1,2,3,4-Tetrahydroanthracene
Heat Capacity 298.15 K, C_p = 247.02 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Entropy 298.15 K, S = 227.12 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 388.0 K, ΔH = 2921 J·mol^{-1}
ΔS = 7.53 J·mol^{-1}·K^{-1}
c,I/liq 373.245 K, ΔH = 19157 J·mol^{-1}
ΔS = 51.33 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation L C666T&&J
Evaluation A

$C_{14}H_{14}$ (c,I) 88MES/FIN
1,2-Diphenylethane
Heat Capacity 298.15 K, C_p = 253.764 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 267.391 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 273.150 K, ΔH = 2247.55 J·mol^{-1}
ΔS = 8.23 J·mol^{-1}·K^{-1}
c,I/liq 324.348 K, ΔH = 22730.52 J·mol^{-1}
ΔS = 70.08 J·mol^{-1}·K^{-1}
Molecular Weight 182.2646
Wiswesser Line Notation R2R
Evaluation A

$C_{14}H_{14}N_2O_3$ (c) 82JAI
p-Azoxyanisole; 4,4′-Dimethoxyazoxybenzene
Phase Changes
c,III/c,I 250.7 K, ΔH = 104.6 J·mol^{-1}
ΔS = 0.42 J·mol^{-1}·K^{-1}
c,II/c,I 335.6 K
c,II/liq 377.5 K, ΔH = 23891 J·mol^{-1}
ΔS = 63.30 J·mol^{-1}·K^{-1}
Crystal II-nematic.
c,I/liq 388.0 K, ΔH = 30430 J·mol^{-1}
ΔS = 78.41 J·mol^{-1}·K^{-1}
Crystal I-nematic.
liq/liq 406.9 K, ΔH = 757 J·mol^{-1}
ΔS = 1.84 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 258.2762
Wiswesser Line Notation 1OR DNUNOR DO1
Evaluation A

$C_{14}H_{16}CrI$ (c) 72NIK/SAF
Bis(toluene)chromium iodide
Heat Capacity 298.15 K, C_p = 333.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 328.2 J·mol^{-1}·K^{-1}
Molecular Weight 363.1809
Wiswesser Line Notation L6ØJ A1 Ø-CR-- ØL6ØJ A1 &I
Evaluation B

$C_{14}H_{16}N_2O_2$ (liq) 86ACH/HAS
1,3-Bis-(1-isocyanato-1-methylethyl)benzene
Heat Capacity 333 K, C_p = 464 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K.
C_p = 1.9 J·g^{-1}·C^{-1}.
Molecular Weight 244.2926
Wiswesser Line Notation OCNX2&1&R CXNCO&2&1
Evaluation C
99% purity.

$C_{14}H_{16}N_2O_2$ (c) 86ACH/HAS
1,4-Bis-(1-isocyanato-1-methylethyl)benzene
Heat Capacity 333 K, C_p = 415 J·mol^{-1}·K^{-1}
Temperature range 333, 433 K.
C_p = 1.7 J·g^{-1}·C^{-1}.
Molecular Weight 244.2926
Wiswesser Line Notation OCNX2&1&R DXNCO&2&1
Evaluation C
99% purity.

$C_{14}H_{18}$ (c) 82GAM/CAL
1,2,3,4,5,6,7,8-Octahydroanthracene
Heat Capacity 298.15 K, C_p = 277.96 J·mol^{-1}·K^{-1}
Temperature range 10 to 400 K.
Entropy 298.15 K, S = 248.92 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 331.348 K, ΔH = 2514.3 J·mol^{-1}
ΔS = 7.59 J·mol^{-1}·K^{-1}
c,I/liq 345.390 K, ΔH = 18341.6 J·mol^{-1}
ΔS = 53.10 J·mol^{-1}·K^{-1}
Molecular Weight 186.2962
Wiswesser Line Notation L 666 T&TJ
Evaluation A

$C_{14}H_{24}$ (c) 82NUZ
Perhydrophenanthrene
Heat Capacity 298 K, C_p = 289.5 J·mol^{-1}·K^{-1}
Temperature range 193 to 403 K.
Phase Changes
c/liq 313 K, ΔH = 11155 J·mol^{-1}
ΔS = 35.64 J·mol^{-1}·K^{-1}
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation B
(cat) cis/anti/trans isomer

$C_{14}H_{24}$ (c) 82NUZ
Perhydrophenanthrene
Heat Capacity 298 K, C_p = 345.6 J·mol^{-1}·K^{-1}
Temperature range 193 to 403 K.
Phase Changes
c/liq 273 K, ΔH = 10481 J·mol^{-1}
ΔS = 38.39 J·mol^{-1}·K^{-1}
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation B
(cst) cis/syn/trans isomer

$C_{14}H_{24}$ (c) 82NUZ
Perhydrophenanthrene
Heat Capacity 298 K, C_p = 281.2 J·mol^{-1}·K^{-1}
Temperature range 193 to 403 K.
Phase Changes
c/liq 283 K, ΔH = 11832 J·mol^{-1}
ΔS = 41.81 J·mol^{-1}·K^{-1}
Molecular Weight 192.3436
Wiswesser Line Notation L B666TJ
Evaluation B
(tat) trans/anti/trans isomer

$C_{14}H_{26}O$ (liq) 87MIL/FEN
2-(1,2-Dimethylpropyl)-5,6-dimethylheptenal
Heat Capacity 323.15 K, C_p = 419.03 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 210.3588
Wiswesser Line Notation 1YYYVH&U2YY
Evaluation A

$C_{14}H_{26}O$ (liq) 87MIL/FEN
2-Pentylnonenal
Heat Capacity 323.15 K, C_p = 435.35 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 428.15 K.
Molecular Weight 210.3588
Wiswesser Line Notation VHY5&U7
Evaluation A

$C_{14}H_{26}O_2$ (liq) 85KAR/ABD
Decyl methacrylate
Heat Capacity 298.15 K, C_p = 452.9 J·mol^{-1}·K^{-1}
Temperature range 250 to 350 K.
Equation only.
C_p (J·kg^{-1}·K^{-1}) = 1098.7 + 3.0251 T.
C_p data calculated from equation.
Phase Changes
c/liq 250.7 K
Molecular Weight 226.3582
Wiswesser Line Notation 10OVY1&U1
Evaluation B

$C_{14}H_{26}O_2$ (liq) 85KAR/ABD2
Decyl methacrylate
Phase Changes
c/liq 250.7 K, ΔH = 30548 J·mol^{-1}
ΔS = 121.9 J·mol^{-1}·K^{-1}
Molecular Weight 226.3582
Wiswesser Line Notation 10OVY1&U1
Evaluation A

$C_{14}H_{27}O_2Tl$ (c) 76MEI/SEY
Thallium tetradecanoate
Phase Changes
c,III/,cII 313 K, ΔH = 11715 J·mol^{-1}
ΔS = 37.2 J·mol^{-1}·K^{-1}
c,II/c,I 371 K, ΔH = 3138 J·mol^{-1}
ΔS = 8.37 J·mol^{-1}·K^{-1}
c,I/liq 393 K, ΔH = 5439 J·mol^{-1}
ΔS = 13.4 J·mol^{-1}·K^{-1}
Solid-mesophase.
liq/liq 460 K, ΔH = 1632 J·mol^{-1}
ΔS = 3.56 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
Molecular Weight 431.7361
Wiswesser Line Notation OV13 .TL
Evaluation B

$C_{14}H_{27}O_2Tl$ (c) 87NGE/WES
Thallium tetradecanoate
Heat Capacity 298.15 K, C_p = 438.25 J·mol^{-1}·K^{-1}
Temperature range 10 to 460 K.
Entropy 298.15 K, S = 473.84 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 318.2 K, ΔH = 15099 J·mol^{-1}
ΔS = 47.39 J·mol^{-1}·K^{-1}
c,II/c,I 378.0 K, ΔH = 2877 J·mol^{-1}
ΔS = 7.65 J·mol^{-1}·K^{-1}
c,I/liq 396.3 K, ΔH = 6269 J·mol^{-1}
ΔS = 15.80 J·mol^{-1}·K^{-1}
Solid-mesomorphic liquid.
Molecular Weight 431.7361
Wiswesser Line Notation OV13 .TL
Evaluation A
Mesomorphic liquid-isotropic liquid phase change data also given:
460.7 K, ΔH = 1671 J·mol^{-1},
ΔS = 3.66 J·mol^{-1}·K^{-1}.

$C_{14}H_{30}$ (liq) 82ZAR
n-Tetradecane
Heat Capacity 298 K, C_p = 436.0 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84GRO/BEN
n-Tetradecane
Heat Capacity 298.15 K, C_p = 436.40 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84GRO/ING
n-Tetradecane
Heat Capacity 298.15 K, C_p = 436.52 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 84ROU/GRO
n-Tetradecane
Heat Capacity 298.15 K, C_p = 436.91 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 85LAI/ROU
n-Tetradecane
Heat Capacity 298.15 K, C_p = 434.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 85LAI/WIL
n-Tetradecane
Heat Capacity 298.15 K, C_p = 434.20 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation A

$C_{14}H_{30}$ (liq) 86WIL/LAI
n-Tetradecane
Heat Capacity 298.15 K, C_p = 433.98 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 88COS/HUU
n-Tetradecane
Heat Capacity 298.15 K, C_p = 438.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation B

$C_{14}H_{30}$ (liq) 88PER/AIC
n-Tetradecane
Heat Capacity 298.15 K, C_p = 438.01 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 198.3910
Wiswesser Line Notation 14H
Evaluation A

$C_{14}H_{30}S$ (liq) 82TUT/GAB
1-Tetradecanethiol; *n*-Tetradecyl mercaptan
Heat Capacity 300 K, C_p = 501.57 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 480.72 + 4.157\times10^{-2}T + 9.310\times10^{-5}T^2$ (J·mol^{-1}·K^{-1})
Molecular Weight 230.4510
Wiswesser Line Notation SH14
Evaluation B

$C_{14}H_{36}N_2CdCl_4$ (c) 83WHI/DAV
Bis(*n*-heptylammonium)tetrachlorocadmate
Heat Capacity 298.15 K, C_p = 633.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 325 K.
Entropy 298.15 K, S = 779.0 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 250.00 K, ΔH = 17630 J·mol^{-1}
ΔS = 71.38 J·mol^{-1}·K^{-1}
c,II/c,I 316.74 K, ΔH = 5060 J·mol^{-1}
ΔS = 16.0 J·mol^{-1}·K^{-1}
Molecular Weight 486.6738
Wiswesser Line Notation 7ZH 2 .CD G4
Evaluation A

$C_{14}H_{36}N_2MgCl_4$ (c) 83WHI/DAV
Bis(*n*-heptylammonium)tetrachloromanganate
Heat Capacity 298.15 K, C_p = 653.0 J·mol^{-1}·K^{-1}
Temperature range 10 to 325 K.
Entropy 298.15 K, S = 772.9 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 247.95 K, ΔH = 16930 J·mol^{-1}
ΔS = 68.2 J·mol^{-1}·K^{-1}
c,II/c,I 313.8 K, ΔH = 10197 J·mol^{-1}
ΔS = 32.5 J·mol^{-1}·K^{-1}
Molecular Weight 398.5688
Wiswesser Line Notation 7ZH 2 .MN G4
Evaluation A

$C_{15}H_{10}N_2O_2$ (c) 77LEB/RAB4
4,4′-Diphenyl methane diisocyanate
Heat Capacity 300 K, C_p = 313 J·mol^{-1}·K^{-1}
Temperature range 13 to 400 K.
Data given graphically.
Value estimated from graph.
Entropy 298.15 K, S = 332.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 313.57 K, ΔH = 27300 J·mol^{-1}
ΔS = 87.1 J·mol^{-1}·K^{-1}
Molecular Weight 250.2562
Wiswesser Line Notation OCNR D1R DNCO
Evaluation C(C_p); A(S,Phase changes)

$(C_{15}H_{10}N_2O_2)_n$ (gls) 77LEB/RAB4
Polyisocyanurate
Heat Capacity 300 K, C_p = 300 J·mol^{-1}·K^{-1}
Temperature range 13 to 400 K.
Data given graphically.
Value estimated from graph.
Entropy 298.15 K, S = 294 J·mol^{-1}·K^{-1}
Molecular Weight 250.2562
Wiswesser Line Notation /T4NVNVTJ A* CR D1R D*/
Evaluation C(C_p), A(S)

$C_{15}H_{12}$ (c) 89CHI/HOS
4-Methylphenanthrene
Heat Capacity 298.15 K, C_p = 263.13 J·mol^{-1}K^{-1}
Temperature range 10 to 500 K.
Entropy 298.15 K, S = 244.55 J·mol^{-1}K^{-1}
Phase Changes
c,III/c,II 182.0 K, ΔH = 22.4 J·mol^{-1}
ΔS = 0.12 J·mol^{-1}·K^{-1}
Extrapolated value.
c,II/c,I 295.0 K, ΔH = 14039 J·mol^{-1}
ΔS = 43.21 J·mol^{-1}·K^{-1}
Molecular Weight 192.2598
Wisweeser Line Notation L B666J C1
Evaluation A

$C_{15}H_{11}N_3O_7$ (c) 79FAR/SHA
Indene picric acid
Phase Changes
c/liq 366.7 K, ΔH = 25100 J·mol^{-1}
ΔS = 68.5 J·mol^{-1}·K^{-1}
Molecular Weight 345.2678
Wiswesser Line Notation L56 BHJ &WNR BQ CNW ENW
Evaluation B

$C_{15}H_{12}$ (c) 88CHI/HOS
4-Methylphenanthrene
Heat Capacity 298.15 K, C_p = 263.13 J·mol^{-1}·K^{-1}
Temperature range 10 to 500 K.
Value is a graphical extrapolation.
Entropy 298.15 K, S = 244.55 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 182.0 K, ΔH = 22.4 J·mol^{-1}
ΔS = 0.12 J·mol^{-1}·K^{-1}
Extrapolated value.
c,II/c,I 295 K, ΔH = 33.3 J·mol^{-1}
ΔS = 0.11 J·mol^{-1}·K^{-1}
Extrapolated value.
c,I/liq 324.925 K, ΔH = 14039 J·mol^{-1}
ΔS = 43.21 J·mol^{-1}·K^{-1}
Molecular Weight 192.2598
Wiswesser Line Notation L B666J C1
Evaluation A

$C_{15}H_{15}Co_3S_2$ (c) 71/SOR/KOS
Tris-(cyclopentadienylcobalt)disulfide
Phase Changes
c,II/c,I 192.5 K, ΔH = 5253.4 J·mol^{-1}
ΔS = 28.894 J·mol^{-1}·K^{-1}
Molecular Weight 436.2031
Wiswesser Line Notation L5ØJ Ø-CO-- 3 &S 2
Evaluation A

$C_{15}H_{15}Y$ (c) 82SHE/KAM
Tricyclopentadienyl yttrium
Heat Capacity 298.15 K, C_p = 289.0 J·mol^{-1}·K^{-1}
Temperature range 4.5 to 300 K.
Entropy 298.15 K, S = 301.6 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 265–280 K
Order-disorder transition.
Molecular Weight 284.1894
Wiswesser Line Notation L5ØJ Ø-Y-- ØL5ØJ &ØL5ØJ
Evaluation A

$C_{15}H_{16}O_2$ (c) 85NOV/TSV
4,4'-Dihydroxydiphenyl-2,2-propane
Heat Capacity 298.15 K, C_p = 287.72 J·mol^{-1}·K^{-1}
Temperature range 14 to 480 K.
Entropy 298.15 K, S = 287.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 433 K, ΔH = 30100 J·mol^{-1}
ΔS = 69.6 J·mol^{-1}·K^{-1}
Molecular Weight 228.2902
Wiswesser Line Notation QR DX1&1&R DQ
Evaluation A

$C_{15}H_{21}AlO_6$ (c) 86GRI/LAZ
Aluminum acetylacetonate
Phase Changes
c/liq 466.7 K, ΔH = 33700 J·mol^{-1}
ΔS = 72.1 J·mol^{-1}·K^{-1}
Molecular Weight 324.3088
Wiswesser Line Notation D6O-AL-O ADJ D1 F1 B-& BD6O-AL-O ADJ D1 F1 B-& BD6O-AL-O ADJ D1 F1
Evaluation A

$C_{15}H_{21}CrO_6$ (c) 86GRI/LAZ
Chromium acetylacetonate
Phase Changes
c/liq 481.9 K, ΔH = 34000 J·mol^{-1}
ΔS = 69.5 J·mol^{-1}·K^{-1}
Molecular Weight 349.3233
Wiswesser Line Notation D6O-CR-O ADJ D1 F1 B-& BD6O-CR-O ADJ D1 F1 B-& BD6O-CR-O ADJ D1 F1
Evaluation A

$C_{15}H_{21}FeO_6$ (c) 87ZHI/KAR
Iron (III) acetylacetonate
Heat Capacity 298.15 K, C_p = 429.9 J·mol^{-1}·K^{-1}
Temperature range 13 to 310 K.
Entropy 298.15 K, S = 526.5 J·mol^{-1}·K^{-1}
Molecular Weight 353.1743
Wiswesser Line Notation D6O-FE-O ADJ D1 F1 B-& BD6O-FE-O ADJ D1 F1 B-& BD6O-FE-O ADJ D1 F1
Evaluation A

$C_{15}H_{26}O_6$ (liq) 86NIL/WAD
Tributyrin; Glyceryl tributyrate
Heat Capacity 298.15 K, C_p = 555.3 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 302.3668
Wiswesser Line Notation 3VO1YOV3&1OV3
Evaluation A

$C_{15}H_{28}O$ (liq) 88BAG/GUR
3,7,11-Trimethyl-1-dodecen-3-ol
Heat Capacity 313.15 K, C_p = 574.4 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 224.3856
Wiswesser Line Notation 1Y3Y3XQ1UU1
Evaluation B

$C_{15}H_{28}O_8$ (liq) 83SAN/CIO
Diethylene glycol-trimethylolpropane-adipate polymer
Heat Capacity 298.15 K, C_p = 636 J·mol^{-1}·K^{-1}
Temperature Range 273.15 to 323.15 K
C_p(kJ kg^{1}·K^{-1}) = 0.016882T - 3.143
Molecular Weight 336.3814
Wiswesser Line Notation /*O2O2OV4VO2Y1Q&20*/
Evaluation D
Authors did not provide formula for repeating unit of polymer; assumed: glycol-adipate-trimethylolpropane, as repeating unit.

$C_{15}H_{32}$ (liq) 81GRO/ING
n-Pentadecane
Heat Capacity 298.15 K, C_p = 467.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 212.4178
Wiswesser Line Notation 15H
Evaluation B

$C_{15}H_{32}$ (liq) 88COS/HUU
n-Pentadecane
Heat Capacity 298.15 K, C_p = 468.81 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 212.4178
Wiswesser Line Notation 15H
Evaluation B

$C_{15}H_{32}O_6$ (liq) 82ZAR
Pentapropylene glycol
Heat Capacity 298 K, C_p = 685.6 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 308.4142
Wiswesser Line Notation QYOYOYOYOYQ
Evaluation B

$(C_{16}H_8D_8)_n$ (gls) 82LEB/SMI
Polystyrene-Polystyrene-d_8 copolymer
Heat Capacity 298.15 K, C_p = 279.1 J·mol^{-1}·K^{-1}
Temperature range 7 to 330 K.
Entropy 298.15 K, S = 291.4 J·mol^{-1}·K^{-1}
Molecular Weight 216.3656
Wiswesser Line Notation /*YR&1*/ &/*YR&1*/ &1/2-BCDEF/4/H-2 8
Evaluation A

$(C_{16}H_{10}Ge)_n$ (gls) 77LEB/RAB
Polydiphenyldiethynylgermanium
Heat Capacity 298.15 K, C_p = 279.4 J·mol^{-1}·K^{-1}
Temperature range 50 to 325 K.
Molecular Weight 274.8650
Wiswesser Line Notation /*1UU1-GE-1UU1&R&R*/
Evaluation B

$C_{16}H_{11}N_3O_7$ (c) 79FAR/SHA
Naphthalene picric acid
Phase Changes
c/liq 426.2 K, ΔH = 34700 J·mol^{-1}
ΔS = 81.4 J·mol^{-1}·K^{-1}
Molecular Weight 357.2788
Wiswesser Line Notation L66J &WNR BQ CNW ENW
Evaluation B

$C_{16}H_{12}Ge$ (c) 75LEB/MIL
Diethynyldiphenylgermane
Heat Capacity 298.15 K, C_p = 305.4 J·mol^{-1}·K^{-1}
Temperature range 8.4 to 326 K.
Deposited in VINITI, No 605-75, 10 March 1975.
Entropy 298.15 K, S = 356.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 319.94 K, ΔH = 20100 J·mol^{-1}
ΔS = 62.80 J·mol^{-1}·K^{-1}
Molecular Weight 276.8608
Wiswesser Line Notation 1UU1-GE-1UU1&R&R
Evaluation A

$C_{16}H_{12}Ge$ (c) 75LEB/MIL2
Diethynyldiphenylgermane
Heat Capacity 300 K, C_p = 307.1 J·mol^{-1}·K^{-1}
Temperature range 8 to 326 K.
Entropy 300 K, S = 358.9 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 319.94 K, ΔH = 20100 J·mol^{-1}
ΔS = 62.80 J·mol^{-1}·K^{-1}
Molecular Weight 276.8608
Wiswesser Line Notation 1UU1-GE-1UU1&R&R
Evaluation A

$C_{16}H_{12}N_7$ (c) 84ABR/BAI
Tetramethylammonium hexacyanotrimethylenecyclopropanide
Heat Capacity 295 K, C_p = 442.6 J·mol^{-1}·K^{-1}
Temperature range 233 to393 K.
Phase Changes
c,II/c,I 363.7 K, ΔH = 1350 J·mol^{-1}
ΔS = 3.4 J·mol^{-1}·K^{-1}
Molecular Weight 302.3177
Wiswesser Line Notation L3YYYJ AU1CN&CN BU1CN&CN CU1CN&CN &K1&1&1
Evaluation B
Treated as a second-order transition, the phase change gives a heat capacity discontinuity of 56 J·mol^{-1}·K^{-1} at 363.7 K.

$C_{16}H_{12}Si$ (c) 77MIL/LEB
Diphenyldiethynylsilane
Heat Capacity 298.15 K, C_p = 381.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 326 K.
Entropy 298.15 K, S = 411.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 209 K, ΔH = 22360 J·mol^{-1}
ΔS = 70.60 J·mol^{-1}·K^{-1}
Crystal-glass transition.
c,I/liq 316.72 K
Molecular Weight 232.3563
Wiswesser Line Notation 1UU1-SI-1UU1&R&R
Evaluation A

$C_{16}H_{15}NO_3$ (c) 87BYK/KIP
3-Phenyl-5-phenoxymethyl-2-oxazolidinone
Heat Capacity 298.15 K, C_p = 310.6 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 330.0 J·mol^{-1}·K^{-1}
Molecular Weight 269.2994
Wiswesser Line Notation T5NVOTJ AR D1OR
Evaluation A

$C_{16}H_{16}$ (c) 73ROD/WES
2,2-Paracyclophane; Cyclo-di-p-xylene
Heat Capacity 298.15 K, C_p = 252.7 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.290 cal·K^{-1}·g^{-1}.
Molecular Weight 208.3024
Wiswesser Line Notation L F6 C-12-6 *A* B F- F--&T&J
Evaluation A

$C_{16}H_{18}$ (c) 83KRA/BEC
2,3-Dimethyl-2,3-diphenylbutane
Heat Capacity 298 K, C_p = 283.4 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.322 Cal.K^{-1}.g^{-1}.
Molecular Weight 210.3182
Wiswesser Line Notation 1XR&XR
Evaluation B

$C_{16}H_{20}CrI$ (c) 72NIK/SAF
Bis(m-xylene)chromium iodide
Heat Capacity 298.15 K, C_p = 353.3 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 370.1 J·mol^{-1}·K^{-1}
Molecular Weight 391.2345
Wiswesser Line Notation L6ØJ A1 C1 Ø-CR-- ØL6ØJ A1 C1 &I
Evaluation B

$C_{16}H_{20}CrI$ (liq) 72NIK/SAF
Bis(ethylbenzene)chromium iodide
Heat Capacity 298.15 K, C_p = 393.3 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 406.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 275.6 K
Molecular Weight 391.2345
Wiswesser Line Notation L6ØJ A2 Ø-CR-- ØL6ØJ A2 &I
Evaluation B
Data also given for glassy phase from 60 to 190 K.

$C_{16}H_{22}OSi_2$ (liq) 83DZH/KUL
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane
Heat Capacity 298.15 K, C_p = 508.1 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Phase Changes
c/liq 250 K
Molecular Weight 286.5202
Wiswesser Line Notation 1-SI-1&R&O-SI-1&1&R
Evaluation A
T(glass) = 167 K.

$C_{16}H_{22}O_3Si_3$ (liq) 87DZH/KUL2
1,1,3,3-Tetraethyl-5,5-diphenylcylotrisiloxane
Heat Capacity 298.15 K, C_p = 629.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 315 K.
Entropy 298.15 K, S = 711.4 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 279.082 K, ΔH = 18374 J·mol^{-1}
ΔS = 66.01 J·mol^{-1}·K^{-1}
Molecular Weight 346.6045
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 ER ER
Evaluation A

$C_{16}H_{22}O_4$ (c) 70MAR/RAB
Dibutyl *o*-phthalate
Heat Capacity 300 K, C_p = 477.0 J·mol^{-1}·K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S = 514.6 J·mol^{-1}·K^{-1}
Molecular Weight 278.3474
Wiswesser Line Notation 4OVR BVO4
Evaluation B
T(glass) = 173.5 °C.

$C_{16}H_{22}O_4$ (liq) 85RAB/NOV
Dibutyl *o*-phthalate
Heat Capacity 298.15 K, C_p = 476.0 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S = 561.1 J·mol^{-1}·K^{-1}
Molecular Weight 278.3474
Wiswesser Line Notation 4OVR BVO4
Evaluation A
Data given for glassy state from 10 to 170 K.
T(glass) = 173.5 K.

$C_{16}H_{24}Si_8O_{12}$ (c) 85PAN/KOZ
Octa(vinylsilasesquioxane)
Heat Capacity 300 K, C_p = 760 J·mol^{-1}·K^{-1}
Temperature range 160 to 300 K.
C_p value estimated from graphical data.
Phase Changes
c,II/c,I 229.6 K, ΔH = 9200 J·mol^{-1}
ΔS = 40.0 J·mol^{-1}·K^{-1}
Molecular Weight 633.0424
Wiswesser Line Notation XXXXXX
Evaluation C(C_p), B(Phase changes)

$C_{16}H_{31}O_2Tl$ (c) 76MEI/SEY
Thallium hexadecanoate
Phase Changes
liq/liq 450 K, ΔH = 1381 J·mol^{-1}
ΔS = 3.05 J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,II/c,I 327 K, ΔH = 10878 J·mol^{-1}
ΔS = 33.5 J·mol^{-1}·K^{-1}
c,I/liq 390 K, ΔH = 8786 J·mol^{-1}
ΔS = 22.2 J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 459.7897
Wiswesser Line Notation OV15 .TL
Evaluation B

$C_{16}H_{34}$ (liq) 88COS/HUU
2,2,4,4,6,8,8-Heptamethylnonane
Heat Capacity 298.15 K, C_p = 458.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 1X1&1&1X1&1&1Y1&1X1&1&1
Evaluation B

$C_{16}H_{34}$ (liq) 88PER/AIC
2,2,4,4,6,8,8-Heptamethylnonane
Heat Capacity 298.15 K, C_p = 458.80 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 1X1&1&1X1&1&1Y1&1X1&1&1
Evaluation A

$C_{16}H_{34}$ (liq) 81GRO/ING
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p = 499.97 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 82ZAR
n-Hexadecane; Cetane
Heat Capacity 298 K, C_p = 498.3 J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 85LAI/ROU
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p = 496.45 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 86TAR/AIC
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p = 499.62 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 86WIL/LAI
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p = 495.73 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 88COS/HUU
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p = 500.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation B

$C_{16}H_{34}$ (liq) 88PER/AIC
n-Hexadecane; Cetane
Heat Capacity 298.15 K, C_p = 500.21 J·mol^{-1}·K^{-1}
One temperature.
Molecular Weight 226.4446
Wiswesser Line Notation 16H
Evaluation A

$C_{16}H_{34}O$ (c) 1889EYK
n-Cetyl alcohol; 1-Hexadecanol
Phase Changes
c/liq 320 K, ΔH = 34727 J·mol^{-1}
ΔS = 108.5 J·mol^{-1}·K^{-1}
Molecular Weight 242.4440
Wiswesser Line Notation Q16
Evaluation C

$C_{16}H_{34}S$ (liq) 82TUT/GAB
1-Hexadecanethiol; *n*-Hexadecyl mercaptan
Heat Capacity 300 K, C_p = 574.22 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 553.16 + 4.153\times10^{-2}T + 9.560\times10^{-5}T^2$.
Molecular Weight 258.5046
Wiswesser Line Notation SH16
Evaluation B

$C_{16}H_{35}N$ (liq) 87MIL/FEN
N,N-Dimethyl-2-pentylnonylamine
Heat Capacity 323.15 K, C_p = 537.98 J·mol^{-1}·K^{-1}
Temperature range 323.15 to 423.15 K.
Molecular Weight 241.4592
Wiswesser Line Notation 7Y5&1N1&1
Evaluation A

$C_{16}H_{36}ClN$ (c) 88VAN/WHI
Di-*n*-octylammonium chloride
Heat Capacity 298.24 K, C_p = 550.2 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 297.70 K, ΔH = 33610 J·mol^{-1}
ΔS = 112.97 J·mol^{-1}·K^{-1}
Molecular Weight 277.9201
Wiswesser Line Notation 8M8 &GH
Evaluation A

$C_{16}H_{36}N_4$ (c) 87KUL/KIP
cis-(5,12)-7,7,14,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane
Heat Capacity 298.15 K, C_p = 444.9 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 443.1 J·mol^{-1}·K^{-1}
Molecular Weight 284.4872
Wiswesser Line Notation L14N DN HN KNTJ E1 G1 G1 L1 N1 N1
Evaluation A

$C_{16}H_{40}O_4Si_4$ (liq) 87DZH/KUL
Octaethylcyclotetrasiloxane
Heat Capacity 298.15 K, C_p = 746.8 J·mol^{-1}·K^{-1}
Temperature range 5 to 300 K.
Entropy 298.15 K, S = 909.3 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 134 K
c,II/c,I 208.16 K, ΔH = 12219 J·mol^{-1}
ΔS = 58.69 J·mol^{-1}·K^{-1}
c,I/liq 213.35 K, ΔH = 13705 J·mol^{-1}
ΔS = 64.38 J·mol^{-1}·K^{-1}
Molecular Weight 408.8316
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A2 A2 C2 C2 E2 E2 G2 G2
Evaluation A

$C_{17}H_{12}$ (c) 79FAR/SHA
2,3-Benzofluorene
Phase Changes
c/liq 489.7 K, ΔH = 23400 J·mol^{-1}
ΔS = 47.8 J·mol^{-1}·K^{-1}
Molecular Weight 216.2818
Wiswesser Line Notation L D6 B656 LHJ
Evaluation B

$C_{17}H_{12}$ (c) 79FAR/SHA
1,2-Benzofluorene
Phase Changes
c,II/c,I 399.9 K, ΔH = 3800 J·mol^{-1}
ΔS = 9.50 J·mol^{-1}·K^{-1}
c/liq 462.8 K, ΔH = 18400 J·mol^{-1}
ΔS = 39.7 J·mol^{-1}·K^{-1}
Molecular Weight 216.2818
Wiswesser Line Notation L D6 B566 CHJ
Evaluation B

$C_{17}H_{14}N_2$ (c) 77LEB/RAB4
2,2-Bis(4-cyanatophenyl)propane
Heat Capacity 300 K, C_p = 360 J·mol^{-1}·K^{-1}
Temperature range 13 to 400 K.
Data given graphically.
Value estimated from graph.
Phase Changes
c/liq 355.8 K, ΔH = 26700 J·mol^{-1}
ΔS = 74.9 J·mol^{-1}·K^{-1}
Molecular Weight 246.3110
Wiswesser Line Notation NCR DX1&1&R DCN
Evaluation C(C_p); A(Phase changes)

$C_{17}H_{14}N_2$ (c) 75LEB/ARO
2,2-Bis-(4-cyanatophenyl)propane
Heat Capacity 298.15 K, C_p = 355.64 J·mol^{-1}·K^{-1}
Temperature range 0 to 420 K.
Entropy 298.15 K, S = 391.2 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 355.83 K, ΔH = 26694 J·mol^{-1}
ΔS = 74.89 J·mol^{-1}·K^{-1}
Molecular Weight 246.3110
Wiswesser Line Notation NCR DX1&1&R DCN
Evaluation A

$(C_{17}H_{14}N_2O_2)_n$ (amorph) 75LEB/ARO
Poly[2,2-bis-(4-phenoxypropane)]2,4,6-triazine; Polycyanate
Heat Capacity 298.15 K, C_p = 326.8 J·mol^{-1}·K^{-1}
Temperature range 0 to 420 K.
Entropy 298.15 K, S = 325.9 J·mol^{-1}·K^{-1}
Molecular Weight 278.3098
Wiswesser Line Notation T6N CN ENJ BOR& DX1&1&RO* DOR& DX1&1&RO* EOR& DX1&1&RO*/ 1/3
Evaluation A

$C_{17}H_{20}Cl_2N_2S$ (c) 83CHA/MAS
Chlorpromazine hydrochloride; 2-Chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene hydrochloride
Phase Changes
c/liq 294.85 K, ΔH = 28420 J·mol^{-1}
ΔS = 60.8 J·mol^{-1}·K^{-1}
Molecular Weight 355.3305
Wiswesser Line Notation T C666 BN ISJ B3N1&1 FG &GH
Evaluation C
(Pre-melting began at 461.7 K).

$C_{17}H_{36}$ (liq) 55SCH/BUS
n-Heptadecane
Phase Changes
c,II/c,I 283.65 K
c,I/liq 294.85 K
Molecular Weight 240.4714
Wiswesser Line Notation 17H
Evaluation B

$C_{18}H_8N_4$ (c) 79BOE/WES
Naphthalene-tetracyanoethylene
Heat Capacity
Temperature range 5 to 300 K.
Data graphically only.
Phase Changes
c,III/c,II 160 K, ΔS = 5.10 J·mol^{-1}·K^{-1}
Bifurcated peak.
Transition region 150 to 172.5 K.
c,II/c,I 222 K, ΔS = 5.02 J·mol^{-1}·K^{-1}
Extended transition.
Transition region 172.5 to 240K.
Molecular Weight 280.2880
Wiswesser Line Notation L66J &NC1U1CN
Evaluation A

$C_{18}H_{11}N_3O_7$ (c) 79FAR/SHA
Acenaphthene picric acid
Phase Changes
c/liq 436.3 K, ΔH = 36000 J·mol^{-1}
ΔS = 82.5 J·mol^{-1}·K^{-1}
Molecular Weight 381.3008
Wiswesser Line Notation L566 1A LT&&J &WNR BQ CNW ENW
Evaluation B

$C_{18}H_{14}$ (c) 83CHA
p-Terphenyl
Heat Capacity 298.15 K, C_p = 278.68 J·mol^{-1}·K^{-1}
Temperature range 4 to 580 K.
$C_p = 35.12 + 0.58825T + 0.0010062T^2 - 8.042\times10^{-7}T^3$ from 80 to 300 K.
Entropy 298.15 K, S = 285.62 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 193.55 K
Lambda transition.
c/liq 487.0 K, ΔH = 35300 J·mol^{-1}
ΔS = 72.5 J·mol^{-1}·K^{-1}
Molecular Weight 230.3086
Wiswesser Line Notation RR DR
Evaluation A

$C_{18}H_{14}$ (c) 82WAS/RAD
p-Terphenyl
Heat Capacity 300 K, C_p = 260 J·mol^{-1}·K^{-1}
Temperature range 180 to 500 K.
Data given graphically.
Value estimated from graph.
Phase Changes
c,II/c,I 400 to 493.1 K
c/liq 493.1 K, ΔH = 41600 J·mol^{-1}
ΔS = 84.4 J·mol^{-1}·K^{-1}
Molecular Weight 230.3086
Wiswesser Line Notation RR DR
Evaluation D(C_p), B(Phase changes)

$C_{18}H_{14}$ (c) 79SMI
p-Terphenyl
Phase Changes
c/liq 486.3 K, ΔH = 35500 J·mol^{-1}
ΔS = 73.0 J·mol^{-1}·K^{-1}
Molecular Weight 230.3086
Wiswesser Line Notation RR DR
Evaluation A

$C_{18}H_{15}ClSi$ (c) 68KOS/MOS
Triphenylchlorosilane
Heat Capacity 298.15 K, C_p = 337.6 J·mol^{-1}·K^{-1}
Temperature range 12.39 to 386.93 K.
Entropy 298.15 K, S = 370.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 370.6 K, ΔH = 26878 J·mol^{-1}
ΔS = 72.53 J·mol^{-1}·K^{-1}
Molecular Weight 294.8550
Wiswesser Line Notation G-SI-R&R&R
Evaluation A

$C_{18}H_{15}OP$ (c) 77HAR/HEA
Triphenylphosphine oxide
Heat Capacity 298.15 K, C_p = 317 J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.14 J·K^{-1}·g^{-1}.
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation B

$C_{18}H_{15}OP$ (c) 78JOR/AIR
Triphenylphosphine oxide
Heat Capacity 298 K, C_p = 470 J·mol^{-1}·K^{-1}
One temperature.
Phase Changes
c/liq 429 K, ΔH = 23800 J·mol^{-1}
ΔS = 55.5 J·mol^{-1}·K^{-1}
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation C

$C_{18}H_{15}OP$ (c) 88KIR/DOM
Triphenylphosphine oxide
Phase Changes
c/liq 431.9 K, $\Delta H = 24220$ J·mol^{-1}
$\Delta S = 56.08$ J·mol^{-1}·K^{-1}
Molecular Weight 278.2897
Wiswesser Line Notation OPR&R&R
Evaluation A

$C_{18}H_{15}O_4P$ (c) 86RAB/PET
Triphenyl phosphate
Heat Capacity 300 K, $C_p = 356.2$ J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 300 K, $S = 397.5$ J·mol^{-1}·K^{-1}
Phase Changes
c/liq 322.55 K, $\Delta H = 29610$ J·mol^{-1}
$\Delta S = 91.80$ J·mol^{-1}·K^{-1}
Molecular Weight 326.2879
Wiswesser Line Notation RO 3 &PO
Evaluation A

$C_{18}H_{15}P$ (c) 88KIR/DOM
Triphenylphosphine
Phase Changes
c/liq 354.4 K, $\Delta H = 19690$ J·mol^{-1}
$\Delta S = 55.56$ J·mol^{-1}·K^{-1}
Molecular Weight 262.2903
Wiswesser Line Notation RPR&R
Evaluation A

$C_{18}H_{16}$ (liq) 78GOO/SCO
4bα,4cβ,5,9bβ,9cα,10-Hexahydrocyclabuta[1,2-a:3,4-a']diindene; anti,*trans*-Truxane
Heat Capacity 298.15 K, $C_p = 252.7$ J·mol^{-1}·K^{-1}
One temperature. $C_p = 0.260$ cal·g^{-1}.
Molecular Weight 232.3244
Wiswesser Line Notation L E6 C5 B456&TTT&J
Evaluation B

$C_{18}H_{16}$ (liq) 78GOO/SCO
4bβ,4cα,9,9aα,9bβ,10-Hexahydrocyclobuta[1,2-a:4,3-a']diindene; syn,*trans*-Truxane
Heat Capacity 298.15 K, $C_p = 275.1$ J·mol^{-1}·K^{-1}
One temperature. $C_p = 0.283$ cal·g^{-1}.
Molecular Weight 232.3244
Wiswesser Line Notation L D6 C5 B456&TTT&J
Evaluation B

$C_{18}H_{18}$ (liq) 78GOO/SCO
2,2'-Biindanyl
Heat Capacity 298.15 K, $C_p = 332.4$ J·mol^{-1}·K^{-1}
One temperature. $C_p = 0.339$ cal·g^{-1}.
Molecular Weight 234.3402
Wiswesser Line Notation L56T&J C- CL56T&J
Evaluation B

$C_{18}H_{18}ClNS$ (c) 83CHA/MAS
Chlorprothixene; 2-Chloro-9-(3-dimethylamino-propylidene)-10-thioxanthene
Phase Changes
c/liq 370.3 K, $\Delta H = 27820$ J·mol^{-1}
$\Delta S = 75.1$ J·mol^{-1}·K^{-1}
Molecular Weight 315.8663
Wiswesser Line Notation T C666 BS IYT EG IU3N1&1
Evaluation C

$C_{18}H_{21}NO$ (liq) 75JAN/JAN
N-(4-Methoxybenzylidene)-*p*-(*n*-butyl)aniline
Heat Capacity 300 K, $C_p = 490$ J·mol^{-1}·K^{-1}
Temperature range 100 to 340 K.
C_p value estimated from graphical data.
Phase Changes
c/liq 295.3 K, $\Delta H = 18033$ J·mol^{-1}
$\Delta S = 61.04$ J·mol^{-1}·K^{-1}
Data also given for metastable modification:
294.0 K, $\Delta H = 14757$ J·mol^{-1}
$\Delta S = 50.21$ J·mol^{-1}·K^{-1}.
Molecular Weight 267.3700
Wiswesser Line Notation 4R DNU1R DO1
Evaluation A(Phase changes), D(C_p)
Phase change data for the metastable modification clearing point also given:
$T = 317.0$ K; $\Delta S = 1.962$ J·mol^{-1}·K^{-1}.

$C_{18}H_{21}NO$ (liq) 82SHI/MIZ
N-(4-Methoxybenzylidene)-*p*-*n*-butylaniline
Heat Capacity 298.15 K, $C_p = 477$ J·mol^{-1}·K^{-1}
Temperature range 293 to 333 K.
Data given graphically.
C_p value is a graphical estimate.
Phase Changes
liq/liq 320.137 K
Nematic-isotropic liquid transition.
Molecular Weight 267.3700
Wiswesser Line Notation 4R DNU1R DO1
Evaluation C

$C_{18}H_{22}N_2O$ (liq) 85SHA/ZHU
4-Ethoxy-4'-butylazobenzene
Heat Capacity 325.49 K, $C_p = 535.0$ J·mol^{-1}·K^{-1}
Temperature range 325 to 363 K.
Unsmoothed experimental datum.
Phase Changes
liq/liq 355.8 K, $\Delta H = 655$ J·mol^{-1}
$\Delta S = 1.84$ J·mol^{-1}·K^{-1}
Molecular Weight 282.3846
Wiswesser Line Notation 4R DNUNR DO2
Evaluation B

$C_{18}H_{24}CrI$ (c) 72NIK/SAF
Bis(mesitylene)chromium iodide
Heat Capacity 298.15 K, $C_p = 437.2$ J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, $S = 443.5$ J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 260 K, $\Delta H = 105$ J·mol^{-1}
$\Delta S = 0.40$ J·mol^{-1}·K^{-1}
Molecular Weight 419.2881
Wiswesser Line Notation L6ØJ A1 C1 D1 Ø-CR-- ØL6ØJ A1 C1 D1 &I
Evaluation B

$C_{18}H_{24}CrI$ (c) 72NIK/SAF
Bis(diisopropylbenzene)chromium iodide
Heat Capacity 298.15 K, $C_p = 633.9$ J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, $S = 569.0$ J·mol^{-1}·K^{-1}
Molecular Weight 419.2881
Wiswesser Line Notation L6ØJ AY DY Ø-CR-- ØL6ØJ AY DY &I
Evaluation B

$C_{18}H_{28}Si_4O_4$ (c) 81MEK/KAR
1,1,3,3,5,5-Hexamethyl-7,7-diphenyltetrasiloxane
Heat Capacity 298.15 K, C_p = 633.0 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Data given graphically.
Entropy 298.15 K, S = 758.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 304.96 K, ΔH = 42731 J·mol^{-1}
ΔS = 140.1 J·mol^{-1}·K^{-1}
Molecular Weight 420.7588
Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-OTJ A1 A1 C1 C1 E1 E1 GR GR
Evaluation A

$C_{18}H_{30}$ (c) 86CHI/ANN
Hexaethylbenzene
Phase Changes
c/g ΔH = 94977 J·mol^{-1}
Molecular Weight 246.4350
Wiswesser Line Notation 2R B2 C2 D2 E2 F2
Evaluation A

$C_{18}H_{30}BaCa_2O_{12}$ (c) 55MOM/SEK
Barium dicalcium propionate
Phase Changes
c/liq 268.4 K, ΔH = 7284 J·mol^{-1}
ΔS = 27.2 J·mol^{-1}·K^{-1}
Molecular Weight 655.9178
Wiswesser Line Notation OV1 6 .BE 4O
Evaluation B

$C_{18}H_{30}Ca_2O_{12}Pb$ (c) 65NAK/SUG
Lead dicalcium propionate
Heat Capacity 298.15 K, C_p = 740.6 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S = 983.2 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 191.5 K, ΔH = 4853 J·mol^{-1}
ΔS = 24.4 J·mol^{-1}·K^{-1}
Molecular Weight 725.7878
Wiswesser Line Notation OV1 6 &-CA- 2 &-PB-
Evaluation A

$C_{18}H_{30}Ca_2O_{12}Sr$ (c) 65NAK/SUG
Strontium dicalcium propionate
Heat Capacity 298.15 K, C_p = 728.4 J·mol^{-1}·K^{-1}
Temperature range 15 to 300 K.
Entropy 298.15 K, S = 949.3 J·mol^{-1}·K^{-1}
Phase Changes
c,III/c,II 104.2 K, ΔH = 1067 J·mol^{-1}
ΔS = 13.4 J·mol^{-1}·K^{-1}
c,II/c,I 282.6 K, ΔH = 667.8 J·mol^{-1}
ΔS = 2.55 J·mol^{-1}·K^{-1}
Molecular Weight 606.2078
Wiswesser Line Notation OV1 6 .CA 2 .SR
Evaluation A

$C_{18}H_{30}O_4$ (c) 77KAR/SAP
p-Diacetylbenzene diethyl ketal
Phase Changes
c,II/c,I 168.2 K, ΔH = 1305 J·mol^{-1}
ΔS = 8.4 J·mol^{-1}·K^{-1}
c,I/liq 326.21 K, ΔH = 23502 J·mol^{-1}
ΔS_m = 23502/326.21 = 72.0 J·mol^{-1}·K^{-1}.
Molecular Weight 310.4326
Wiswesser Line Notation 2OXO2&1&R DX1&O2&O2
Evaluation A
T(glass) = 208.0 K, see also 78KAR/SAP.

$C_{18}H_{30}O_4$ (c) 78KAR/SAP
p-Diacetylbenzene diethyl ketal
Heat Capacity 300 K, C_p = 460 J·mol^{-1}·K^{-1}
Temperature range 5 to 326.1 K.
Data given graphically.
Value estimated from graph.
Entropy 298.15 K, S = 493.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 168.2 K, ΔH = 1307 J·mol^{-1}
ΔS = 8.15 J·mol^{-1}·K^{-1}
c,I/liq 326.21 K, ΔH = 23500 J·mol^{-1}
ΔS = 72.04 J·mol^{-1}·K^{-1}
Molecular Weight 310.4326
Wiswesser Line Notation 2OXO2&1&R DX1&O2&O2
Evaluation C(C_p), A(S,Phase changes)
T(glass) = 208.0 K.

$C_{18}H_{30}O_4$ (c) 78KAR/RAB
p-Diacetylbenzene diethyl ketal
Heat Capacity 298.15 K, C_p = 462.0 J·mol^{-1}·K^{-1}
Temperature range 5 to 340 K.
Entropy 298.15 K, S = 493.8 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 168.24 K, ΔH = 1307 J·mol^{-1}
ΔS = 8.14 J·mol^{-1}·K^{-1}
c,I/liq 326.61 K, ΔH = 23500 J·mol^{-1}
ΔS = 71.95 J·mol^{-1}·K^{-1}
Molecular Weight 310.4326
Wiswesser Line Notation 2OXO2&1&R DX1&O2&O2
Evaluation A
Glass transition at T(glass) = 208 K.

$C_{18}H_{32}O$ (liq) 88BAG/GUR
6,10,14-Trimethyl-3,5-pentadecadien-2-one
Heat Capacity 293.95 K, C_p = 555.3 J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 264.4502
Wiswesser Line Notation 1Y3Y3YU2U1V1
Evaluation B

$C_{18}H_{34}O_3$ (liq) 84URY/MOC
Castor oil; Natural ricinoleic acid
Heat Capacity 300 K, C_p = 646 J·mol^{-1}·K^{-1}
Temperature range 80 to 320 K.
Entropy 300 K, S = 620 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 205 K
Glass transition;
ΔC_p = 0.55 J·g^{-1}·K^{-1} for glass to supercooled liquid transition.
c/liq 264.87 K, ΔH = 17016 J·mol^{-1}
ΔS = 64.2 J·mol^{-1}·K^{-1}
Molecular Weight 298.4648
Wiswesser Line Notation QV8U2YQ6
Evaluation B
General difference in enthalpy of glassy and crystalline phases at T = 0 K is 31.7 J·g^{-1} (9397 J·mol^{-1}).
Entropy of the glassy phase at
T = 0 K is 0.097 J·g^{-1}·K^{-1} (28.8 J·mol^{-1}·K^{-1}).
Castor oil is about 88% ricinoleic acid.

$C_{18}H_{35}O_2Tl$ (c) 76MEI/SEY
Thallium octadecanoate
Phase Changes
liq/liq 444 K, $\Delta H = 1381$ J·mol^{-1}
$\Delta S = 3.05$ J·mol^{-1}·K^{-1}
Mesophase-isotropic.
c,III/c,II 324 K, $\Delta H = 9623$ J·mol^{-1}
$\Delta S = 29.3$ J·mol^{-1}·K^{-1}
c,II/c,I 380 K, $\Delta H = 12134$ J·mol^{-1}
$\Delta S = 12.1$ J·mol^{-1}·K^{-1}
c,I/liq 385 K, $\Delta H = 5439$ J·mol^{-1}
$\Delta S = 14.2$ J·mol^{-1}·K^{-1}
Solid-mesophase.
Molecular Weight 487.8433
Wiswesser Line Notation OV17 .TL
Evaluation B

$C_{18}H_{36}$ (c) 69BOR/DAL
Cyclooctadecane
Phase Changes
c,II/c,I 298 K, $\Delta H = 29288$ J·mol^{-1}
$\Delta S = 97.5$ J·mol^{-1}·K^{-1}
c/liq 346 K, $\Delta H = 9874$ J·mol^{-1}
$\Delta S = 28.4$ J·mol^{-1}·K^{-1}
Molecular Weight 252.4824
Wiswesser Line Notation L-18-TJ
Evaluation B

$C_{18}H_{36}O$ (liq) 88BAG/GUR
6,10,14-Trimethyl-2-pentadecanone; Phytone
Heat Capacity 293.85 K, $C_p = 593.3$ J·mol^{-1}·K^{-1}
Temperature range 270 to 340 K.
Unsmoothed experimental datum.
Molecular Weight 268.4818
Wiswesser Line Notation 1Y3Y3Y3V1
Evaluation B

$C_{18}H_{36}O_2$ (c) 1889EYK
Octadecanoic acid; Stearic acid
Phase Changes
c/liq 326.1 K, $\Delta H = 64643$ J·mol^{-1}
$\Delta S = 198$ J·mol^{-1}·K^{-1}
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation C

$C_{18}H_{36}O_2$ (c) 83BEC/ROU
Octadecanoic acid; Stearic acid
Phase Changes
c/liq 345, 346 K, $\Delta H = 62600$ J·mol^{-1}
$\Delta S = 181$ J·mol^{-1}·K^{-1}
First peak due to pre-melting or dissociation.
Molecular Weight 284.4812
Wiswesser Line Notation QV17
Evaluation B

$C_{18}H_{38}$ (c) 55SCH/BUS
n-Octadecane
Phase Changes
c,I/liq 301.35 K, $\Delta H = 61379$ J·mol^{-1}
$\Delta S = 203.6$ J·mol^{-1}·K^{-1}
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation B

$C_{18}H_{38}$ (liq) 81HOE
n-Octadecane
Heat Capacity 325 K, $C_p = 568$ J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K.
Cv = 2.20 J·g^{-1}·K^{-1}.
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation B

$C_{18}H_{38}$ (c) 85KOL/SYU
n-Octadecane
Phase Changes
c/liq 301.0 K, $\Delta H = 60760$ J·mol^{-1}
$\Delta S = 201.9$ J·mol^{-1}·K^{-1}
Molecular Weight 254.4982
Wiswesser Line Notation 18H
Evaluation A

$C_{18}H_{38}O_7$ (liq) 82ZAR
Hexapropylene glycol
Heat Capacity 298 K, $C_p = 807.4$ J·mol^{-1}·K^{-1}
Temperature range 298, 323, 363 K.
Molecular Weight 366.4940
Wiswesser Line Notation QYOYOYOYOYOYQ
Evaluation B

$C_{18}H_{38}S$ (liq) 82TUT/GAB
1-Octadecanethiol; *n*-Octadecyl mercaptan
Heat Capacity 300 K, $C_p = 648.61$ J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 626.52 + 4.423\times10^{-2}T + 9.800\times10^{-5}T^2$.
Molecular Weight 286.5582
Wiswesser Line Notation SH18
Evaluation B

$C_{19}H_{13}N_3O_7$ (c) 79FAR/SHA
Fluorene picric acid
Phase Changes
c/liq 350.3 K, $\Delta H = 26800$ J·mol^{-1}
$\Delta S = 76.5$ J·mol^{-1}·K^{-1}
Molecular Weight 395.3276
Wiswesser Line Notation L B656 HHJ &WNR BQ CNW ENW
Evaluation B

$C_{19}H_{14}N_2$ (c) 74KAR/RAB
1,2-Diphenylbenzimidazole
Heat Capacity 298.15 K, $C_p = 318.7$ J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 306.8$ J·mol^{-1}·K^{-1}
Molecular Weight 270.3330
Wiswesser Line Notation T56 BN DNJ CR DR
Evaluation A

$C_{19}H_{16}N_2O$ (c) 74KAR/RAB
N-Benzoyl-o-aminodiphenylamine
Heat Capacity 298.15 K, $C_p = 356.6$ J·mol^{-1}·K^{-1}
Temperature range 10 to 450 K.
Entropy 298.15 K, $S = 340.7$ J·mol^{-1}·K^{-1}
Molecular Weight 288.3482
Wiswesser Line Notation RVMR BMR
Evaluation A

$C_{19}H_{20}N_2O_3$ (c) 83FAN/POE

4-Propionyl-4′-*n*-butanoyloxyazobenzene

Phase Changes

c/liq 366 K, ΔH = 15021 J·mol^{-1}
ΔS = 41.04 J·mol^{-1}·K^{-1}

Mesophase observed between 366 and 393 K.

Solid-smectic *H* or G.

Molecular Weight 324.3786

Wiswesser Line Notation 3VOR DNUNR DV2

Evaluation A

Smectic *H* or G-smectic A; smectic A-nematic; nematic-isotropic liquid phase change data also given: 392.65 K, ΔH = 10920 J·mol^{-1}; 409.65 K, ΔH = 4100 J·mol^{-1}; 428.65 K, ΔH = 753 J·mol^{-1}.

$C_{19}H_{22}ClNO$ (c) 82TSU/SOR2

p-*n*-Hexyloxybenzylideneamino-*p*′-chlorobenzene

Heat Capacity 298.15 K, C_p = 434.94 J·mol^{-1}·K^{-1}

Temperature range 15 to 385 K.

Entropy 298.15 K, S = 447.58 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 327.7 K, ΔH = 10880 J·mol^{-1}
ΔS = 33.2 J·mol^{-1}·K^{-1}

Crystal to intermediate phase S_3.

Molecular Weight 315.8419

Wiswesser Line Notation GR DNU1R DO6

Evaluation A

S_3-smectic B; smectic B-smectic A; smectic A-isotropic liquid phase change data also given: 333.90 K, ΔH = 12350 J·mol^{-1}, ΔS = 37.0 J·mol^{-1}·K^{-1}; 362.98 K, ΔH = 3390 J·mol^{-1}, ΔS = 9.3 J·mol^{-1}·K^{-1}; 370.38 K, ΔH = 5790 J·mol^{-1}, ΔS = 15.6 J·mol^{-1}·K^{-1}.

$C_{19}H_{22}FNO$ (c) 82TSU/SOR3

p-*n*-Hexyloxybenzylideneamino-*p*′-fluorobenzene

Heat Capacity 298.15 K, C_p = 442.55 J·mol^{-1}·K^{-1}

Temperature range 15 to 385 K.

Entropy 298.15 K, S = 438.76 J·mol^{-1}·K^{-1}

Phase Changes

c/liq 328.07 K, ΔH = 23220 J·mol^{-1}
ΔS = 70.7 J·mol^{-1}·K^{-1}

Crystal to smectic B.

Molecular Weight 299.3873

Wiswesser Line Notation FR DNU1R DO6

Evaluation A

Smectic B-smectic A; smectic A-nematic; nematic-isotropic liquid phase change data also given: 330.33 K, ΔH = 3050 J·mol^{-1}, ΔS = 9.2 J·mol^{-1}·K^{-1}; 334.88 K, ΔH = 3410 J·mol^{-1}, ΔS = 10.2 J·mol^{-1}·K^{-1}; 336.33 K, ΔH = 1170 J·mol^{-1}, ΔS = 3.5 J·mol^{-1}·K^{-1}.

$C_{19}H_{23}NO$ (c) 73SOR/NAK

N-*p*-Ethoxybenzylidene-*p*′-butylaniline

Heat Capacity 300 K, C_p = 425 J·mol^{-1}·K^{-1}

Temperature range 14 to 375 K.

Data estimated from graph.

Phase Changes

liq/liq 349.08 K, ΔH = 1553 J·mol^{-1}
ΔS = 4.524 J·mol^{-1}·K^{-1}

Nematic-isotropic.

c/liq 305.62 K, ΔH = 27090 J·mol^{-1}
ΔS = 88.71 J·mol^{-1}·K^{-1}

Solid-nematic.

Molecular Weight 281.3968

Wiswesser Line Notation 4R DNU1R DO2

Evaluation B

$C_{19}H_{23}NO$ (c) 74SOR/NAK

N-*p*-Ethoxybenzylidene-*p*′-butylaniline

Heat Capacity 298.15 K, C_p = 429.09 J·mol^{-1}·K^{-1}

Temperature Range 14 to 375 K,

Entrop 298.15 K, ΔS = 421.788 J·mol^{-1}·K^{-1}

Phase Changes

c/nematic liq 305.62 K, ΔH = 27090 J·mol^{-1}
ΔS = 88.71 J·mol^{-1}·K^{-1}

Crystal-nematic

liq/liq 349.08 K, ΔH = 1553 J·mol^{-1}
ΔS = 4.524 J·mol^{-1}·K^{-1}

Nematic-isotropic

Molecular Weight 281.3968

Wiswesser Line Notation 4R DNUIR DO2

Evaluation A

$C_{19}H_{23}NO$ (c) 82TSU/SOR

p-*n*-Hexyloxybenzylideneaniline

Heat Capacity 298.15 K, C_p = 404.52 J·mol^{-1}·K^{-1}

Temperature range 16 to 385 K.

Entropy 298.15 K, S = 424.16 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 73.41 K, ΔH = 192 J·mol^{-1}
ΔS = 2.70 J·mol^{-1}·K^{-1}

c,I/liq 321.63 K, ΔH = 309100 J·mol^{-1}
ΔS = 96.1 J·mol^{-1}·K^{-1}

Solid-isotropic liquid.

Molecular Weight 281.3968

Wiswesser Line Notation 6OR D1UNR

Evaluation A

$C_{19}H_{40}$ (c) 55SCH/BUS

n-Nonadecane

Phase Changes

c,II/c,I 295.95 K, ΔH = 13807 J·mol^{-1}
ΔS = 46.7 J·mol^{-1}·K^{-1}

c,I/liq 305.15 K, ΔH = 45815 J·mol^{-1}
ΔS = 150.1 J·mol^{-1}·K^{-1}

Molecular Weight 268.5250

Wiswesser Line Notation 19H

Evaluation B

$C_{19}H_{40}$ (c) 79CLA/LET

n-Nonadecane

Phase Changes

c,II/c,I 295.95 K, ΔH = 13665 J·mol^{-1}
ΔS = 46.2 J·mol^{-1}·K^{-1}

c,I/liq 303.95 K, ΔH = 47395 J·mol^{-1}
ΔS = 155.9 J·mol^{-1}·K^{-1}

Molecular Weight 268.5250

Wiswesser Line Notation 19H

Evaluation B

$C_{20}H_{10}N_4$ (c) 79BOE/WES
Naphthalene-tetracyanobenzene
Heat Capacity
Temperature range 30 to 80 K.
Data given graphically only.
Phase Changes
c,II/c,I 70 K, $\Delta S = 2.97$ J·mol^{-1}·K^{-1}
Transition extends over 50 K region, abruptly ending at 70 K.
Molecular Weight 306.3258
Wiswesser Line Notation L66J &NCR BCN DCN ECN
Evaluation A

$C_{20}H_{11}Cl_4NO_2$ (c) 87ECO/BER
AnthraceneTCNB; Anthracene-1,2,4,5-tetrachloro-3-nitrobenzene
Heat Capacity
Temperature range 140 to 240 K.
Data given graphically.
Phase Changes
c,III/c,II 208.5 K
c,II/c,I 211.5 K, $\Delta H = 151$ J·mol^{-1}
$\Delta S = 0.71$ J·mol^{-1}·K^{-1}
Total enthalpy and entropy between 180 and 215 K.
Molecular Weight 439.1244
Wiswesser Line Notation WNR BG CG EG FG & L C666J
Evaluation B

$C_{20}H_{13}N_3O_7$ (c) 79FAR/SHA
Anthracene picric acid
Phase Changes
c,II/c,I 364.0 K, $\Delta H = 10500$ J·mol^{-1}
$\Delta S = 28.8$ J·mol^{-1}·K^{-1}
c/liq 417.6 K, $\Delta H = 24300$ J·mol^{-1}
$\Delta S = 58.2$ J·mol^{-1}·K^{-1}
Molecular Weight 407.3386
Wiswesser Line Notation L C666J &WNR BQ CNW ENW
Evaluation B

$C_{20}H_{14}$ (c) 73ROD/WES
Triptycene; 9,10-o-Benzeno-9,10-dihydroanthracene
Heat Capacity 298.15 K, $C_p = 283.1$ J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.266 cal·K^{-1}·g^{-1}.
Molecular Weight 254.3306
Wiswesser Line Notation L 6 H66 O66/GT 2AF T GH NHJ
Evaluation A

$C_{20}H_{14}$ (c) 79FAR/SHA
β,β'-Binaphthyl
Phase Changes
c/liq 461.2 K, $\Delta H = 38900$ J·mol^{-1}
$\Delta S = 84.4$ J·mol^{-1}·K^{-1}
Molecular Weight 254.3306
Wiswesser Line Notation L66J A- AL66J
Evaluation B

$C_{20}H_{14}O_4$ (c) 84OZC/ASR
4,4'-Diethanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 449 K, $\Delta H = 7110$ J·mol^{-1}
$\Delta S = 15.86$ J·mol^{-1}·K^{-1}
c,II/c,I 488 K, $\Delta H = 40200$ J·mol^{-1}
$\Delta S = 62.38$ J·mol^{-1}·K^{-1}
Molecular Weight 318.3282
Wiswesser Line Notation 1VOR DIUU2UU1R DOV1
Evaluation A
First heating, gradual decomposition observed on cycling.

$C_{20}H_{14}O_4$ (c) 84GRA/AVR
Phenolphthalein
Heat Capacity
Temperature range 300 to 550 K.
Data given graphically.
Phase Changes
c,II/c,I 411 K, $\Delta H = 22594$ J·mol^{-1}
$\Delta S = 55.0$ J·mol^{-1}·K^{-1}
Amorphous/crystal.
c/liq 534 K, $\Delta H = 51045$ J·mol^{-1}
$\Delta S = 95.6$ J·mol^{-1}·K^{-1}
Molecular Weight 318.3282
Wiswesser Line Notation T56 BVOT&J DR DQ DR DQ
Evaluation B

$C_{20}H_{16}Fe_2I_3$ (c) 87SOR/NIS
Biferrocenium triiodide
Heat Capacity 300 K, $C_p = 463.72$ J·mol^{-1}·K^{-1}
Temperature range 14 to 360 K.
Interpolated data.
Phase Changes
c,II/c,I 358.675 K, $\Delta H = 538$ J·mol^{-1}
$\Delta S = 1.77$ J·mol^{-1}·K^{-1}
Molecular Weight 748.7539
Wiswesser Line Notation L5ØJ Ø-FE- - ØL5ØJ A- AL5ØJØ-FE- - ØL5ØJ &I3
Evaluation A

$C_{20}H_{18}Sn$ (c) 85CAR/LAY
Triphenyl vinyl tin
Heat Capacity 298.15 K, $C_p = 486.4$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 1.29 J·K^{-1}·g^{-1}.
Molecular Weight 377.0522
Wiswesser Line Notation 1U1-SN-R&R&R
Evaluation B

$C_{20}H_{20}$ (liq) 78GOO/SCO
5,6,6a,6b,11,12,12a,12b-Octahydrodibenzo-[a,g]biphenylene
Heat Capacity 298.15 K, $C_p = 323.6$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.297 cal·g^{-1}.
Molecular Weight 260.3780
Wiswesser Line Notation L F6 C6 B466 &TTT&J
Evaluation B

$C_{20}H_{20}$ (liq) 78GOO/SCO
5,6,6a,6b,7,8,12b,12c-Octahydrodibenzo-[a,i]biphenylene
Heat Capacity 298.15 K, $C_p = 333.4$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.306 cal·g^{-1}.
Molecular Weight 260.3780
Wiswesser Line Notation L D6 C6 B466 &TTT&J
Evaluation B

$C_{20}H_{22}$ (liq) 78GOO/SCO
2,2'-Bitetralin
Heat Capacity 298.15 K, $C_p = 379.9$ J·mol^{-1}·K^{-1}
One temperature. C_p given as 0.346 cal·g^{-1}.
Molecular Weight 262.3938
Wiswesser Line Notation L66T&J C- CL66TT&J
Evaluation B

$C_{20}H_{22}N_2O$ (c) 79TSU/SOR

p-n-Hexyloxybenzylideneamino-*p'*-benzonitrile

Heat Capacity 298.15 K, C_p = 432.51 J·mol^{-1}·K^{-1}

Temperature range 15 to 385 K.

Entropy 298.15 K, S = 450.56 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 306.98 K, ΔH = 5110 J·mol^{-1}

ΔS = 16.7 J·mol^{-1}·K^{-1}

c,I/liq 334.05 K, ΔH = 23770 J·mol^{-1}

ΔS = 71.2 J·mol^{-1}·K^{-1}

Solid nematic.

Molecular Weight 306.4066

Wiswesser Line Notation NCR DNU1R DO6

Evaluation A

Nematic-isotropic liquid phase data also given:

375.10 K, ΔH = 1750 J·mol^{-1},

ΔS = 3.2 J·mol^{-1}·K^{-1}

(Note: 1750/375.10 = 4.67 J·mol^{-1}·K^{-1}).

$C_{20}H_{24}N_2O_3$ (liq) 85SHA/ZHU

4-Methyoxy-4'-heptanoylazobenzene

Heat Capacity 351.84 K, C_p = 685.9 J·mol^{-1}·K^{-1}

Temperature range 351 to 374 K.

Unsmoothed experimental datum.

Phase Changes

liq/liq 371.6 K, ΔH = 573 J·mol^{-1}

ΔS = 1.54 J·mol^{-1}·K^{-1}

Molecular Weight 340.4212

Wiswesser Line Notation 6VOR DNUNR DO1

Evaluation B

$C_{20}H_{25}NO$ (c) 82TSU/SOR4

p-n-Hexyloxybenzylidene-*p'*-toluidine

Heat Capacity 298.15 K, C_p = 441.40 J·mol^{-1}·K^{-1}

Temperature range 17 to385 K.

Entropy 298.15 K, S = 448.95 J·mol^{-1}·K^{-1}

Phase Changes

c,II/c,I 317.5 K, ΔH = 5040 J·mol^{-1}

ΔS = 15.89 J·mol^{-1}·K^{-1}

Superheating phenomenon occurs at 324 K.

c,I/liq 334.26 K, ΔH = 25040 J·mol^{-1}

ΔS = 74.90 J·mol^{-1}·K^{-1}

Solid-nematic.

Molecular Weight 295.4236

Wiswesser Line Notation 60R D1UNR D1

Evaluation A

Nematic-isotropic liquid phase change data also given:

346.90 K, ΔH = 1370 J·mol^{-1},

ΔS = 3.0 J·mol^{-1}·K^{-1}.

$C_{20}H_{26}O$ (c) 79LEW/ENE

Northindrone

Phase Changes

c/liq 479 K, ΔH = 39600 J·mol^{-1}

ΔS = 82.7 J·mol^{-1}·K^{-1}

Molecular Weight 282.4248

Wiswesser Line Notation L E5 B666 OV MUTJ E1 FQ F1UU1

Evaluation A

$C_{20}H_{28}ZrO_6$ (c) 86GRI/LAZ

Zirconium acetylacetonate

Phase Changes

c/liq 470.8 K, ΔH = 50100 J·mol^{-1}

ΔS = 106.3 J·mol^{-1}·K^{-1}

Molecular Weight 455.6576

Wiswesser Line Notation D6O-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1 B-& BD60-ZR-O ADJ D1 F1 B-& BD6O-ZR-O ADJ D1 F1

Evaluation A

$C_{20}H_{33}Cl_2FeN_6O$ (c) 85KAJ/SOR

Tris(2-picolylamine)iron chloride ethanolate

Heat Capacity 300 K, C_p = 590 J·mol^{-1}·K^{-1}

Temperature range 13 to 315 K.

Data graphically only.

Value estimated from graph.

Phase Changes

c,III/c,II 114.04 K

c,II/c,I 122.21 K, ΔH = 6140 J·mol^{-1}

ΔS = 50.59 J·mol^{-1}·K^{-1}

Total transition enthalpy and entropy.

Molecular Weight 500.2734

Wiswesser Line Notation T6NJ B1ZH 3 .FE G2 &G2

Evaluation $C_p(C)$, transitions(A)

$C_{20}H_{40}O$ (liq) 88BAG/GUR

3,7,11,15-Tetramethyl-1-hexadecen-3-ol; Isophytol

Heat Capacity 293.75 K, C_p = 729.5 J·mol^{-1}·K^{-1}

Temperature range 270 to 340 K.

Unsmoothed experimental datum.

Molecular Weight 296.5354

Wiswesser Line Notation 1Y3Y3Y3XQ1U1

Evaluation B

$C_{20}H_{40}O$ (liq) 88BAG/GUR

3,7,11,15-Tetramethyl-1-hexadecyn-3-ol

Heat Capacity 293.85 K, C_p = 712.7 J·mol^{-1}·K^{-1}

Temperature range 270 to 340 K.

Unsmoothed experimental datum.

Molecular Weight 296.5354

Wiswesser Line Notation 1Y3Y3Y3XQ1UU1

Evaluation B

$C_{20}H_{41}NO$ (liq) 81ARU/DAU

4-Octyl-4'-heptyl-α-cyanostilbene

Heat Capacity

Temperature range 320 to 340 K.

Data given graphically.

Molecular Weight 311.5500

Wiswesser Line Notation 8OR D1U1R DYCN&6

Evaluation C

Smectic C-smectic A, 324.3 K;

smectic A-nematic, 337.3 K, ΔS = 1.66 J·mol^{-1}·K^{-1};

nematic-isotropic liquid, 338.5 K, ΔS = 6.98 J·mol^{-1}·K^{-1}

phase change data given. Assume trans isomer.

$C_{20}H_{42}$ (c) 55SCH/BUS

n-Eicosane

Phase Changes

c,II/c,I 309.35 K

c,I/liq 309.75 K, ΔH = 69873 J·mol^{-1}

ΔS = 225.6 J·mol^{-1}·K^{-1}

Molecular Weight 282.5518

Wiswesser Line Notation 20H

Evaluation B

$C_{20}H_{42}$ (c) 73COM

n-Eicosane

Phase Changes

c/liq 309.75 K, ΔH = 69873 J·mol^{-1}

ΔS = 225.6 J·mol^{-1}·K^{-1}

Molecular Weight 282.5518

Wiswesser Line Notation 20H

Evaluation B

$C_{20}H_{42}$ (c) 84SYU/TUM
n-Eicosane
Phase Changes
c/liq 308.5 K, ΔH = 70900 J·mol^{-1}
ΔS = 229.8 J·mol^{-1}·K^{-1}
Relative error in determination ± 5%.
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation B

$C_{20}H_{42}$ (c) 85KOL/SYU
n-Eicosane
Phase Changes
c/liq 308.8 K, ΔH = 67800 J·mol^{-1}
ΔS = 219.6 J·mol^{-1}·K^{-1}
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation A

$C_{20}H_{42}$ (liq) 81HOE
n-Eicosane
Heat Capacity 325 K, C_p = 664 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K.
Cv = 2.32 J·g^{-1}·K^{-1}.
Molecular Weight 282.5518
Wiswesser Line Notation 20H
Evaluation B

$C_{20}H_{42}S$ (liq) 82TUT/GAB
1-Eicosanethiol; *n*-Eicosanyl mercaptan
Heat Capacity 300 K, C_p = 725.84 J·mol^{-1}·K^{-1}
Temperature range 273 to 373 K.
$C_p = 702.70 + 4.703\times10^{-2}T + 10.040\times10^{-5}T^2$.
Molecular Weight 314.6118
Wiswesser Line Notation SH20
Evaluation B

$C_{20}H_{44}ClN$ (c) 88VAN/WHI
Di-*n*-decylammonium chloride
Heat Capacity 297.93 K, C_p = 631.9 J·mol^{-1}·K^{-1}
Temperature range 25 to 350 K.
Unsmoothed experimental datum.
Phase Changes
c,III/c,II 320.13 K
c,II/c,I 321.50 K, ΔH = 50590 J·mol^{-1}
ΔS = 158.97 J·mol^{-1}·K^{-1}
ΔH, ΔS combined data.
Molecular Weight 334.0273
Wiswesser Line Notation 10M10 &GH
Evaluation A

$C_{20}H_{48}Cl_4MnN_2$ (c) 75BOC/ARR
Tetrachlorobis-(decylammonium) manganese II
Phase Changes
c,III/c,II 309 K, ΔH = 1937 J·mol^{-1}
ΔS = 6.3 J·mol^{-1}·K^{-1}
c,II/c,I 437 K, ΔH = 16.8 J·mol^{-1}
ΔS = 0.038 J·mol^{-1}·K^{-1}
Molecular Weight 513.3626
Wiswesser Line Notation 10ZH 2 .MN G4
Evaluation A

$C_{20}.84H_{16}.66O_{0}.62$ (c) 78KAR/SAP
Polyphenylene PP-1
Heat Capacity 300 K, C_p = 280 J·mol^{-1}·K^{-1}
Temperature range 100 to 600 K.
Data given graphically.
Value estimated from graph.
Entropy 298.15 K, S = 253.0 J·mol^{-1}·K^{-1}
Molecular Weight 277.0205
Wiswesser Line Notation /*R DR C* ER/
Evaluation C
WLN excludes ketal end groups and use the repeating unit: $(C_{18}H_{12})_n$.

$C_{20}.84H_{16}.66O_{0}.62$ (c) 78KAR/SAP
Polyphenylene PP-2
Heat Capacity 300 K, C_p = 230 J·mol^{-1}·K^{-1}
Temperature range 100 to 600 K.
Data given graphically.
Value estimated from graph.
Entropy 298.15 K, S = 222.5 J·mol^{-1}·K^{-1}
Molecular Weight 277.0205
Wiswesser Line Notation /*R DR C* ER/
Evaluation C
WLN excludes ketal end groups and use the repeating unit: $(C_{18}H_{12})_n$. PP-2 is the product of thermal crosslinking of PP-1.

$(C_{21}H_{12}N_2O_2)_n$ (c) 75KAR/RAB
Poly-2,2′-(m-phenylene)-5,5′-dibenzoxazole methane
Heat Capacity
Temperature range 60 to 350 K.
Data given graphically.
Entropy 300 K, S = 330.3 J·mol^{-1}·K^{-1}
Molecular Weight 324.3381
Wiswesser Line Notation /T56 BN DOJ C* H1- HT56 BN DOJ CR& C*/
Evaluation A

$C_{21}H_{15}N_3$ (c) 84LEB/BYK2
Triphenyl-s-triazine
Heat Capacity 298.15 K, C_p = 345.1 J·mol^{-1}·K^{-1}
Temperature range 18 to 330 K.
Entropy 298.15 K, S = 349.6 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 506.65 K
Molecular Weight 309.3696
Wiswesser Line Notation T6N CN ENJ BR DR FR
Evaluation A

$(C_{21}H_{16}N_2O_4)_n$ (c) 75KAR/RAB
Poly-4,4′-dihydroxy-3,3′-isophthalamidodiphenylmethane
Heat Capacity
Temperature range 60 to 350 K.
Data given graphically.
Entropy 300 K, S = 448.1 J·mol^{-1}·K^{-1}
Molecular Weight 360.3685
Wiswesser Line Notation /*VMR BQ EIR DQ CMVR C*/
Evaluation A

$C_{21}H_{21}O_4P$ (gls) 86OVC/POD
Tricresyl phosphate
Heat Capacity 298.15 K, C_p = 578 J·mol^{-1}·K^{-1}
Temperature range 6 to 320 K.
Entropy 298.15 K, S = 570 J·mol^{-1}·K^{-1}
Molecular Weight 368.3683
Wiswesser Line Notation OPOR D1 &OR D1 &OR D1
Evaluation A
T(glass) = 207.0 K.

$C_{21}H_{24}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-hexanoyloxyazobenzene
Phase Changes
c/liq 372.15 K, ΔH = 29790 J·mol^{-1}
Solid-smectic A.
Molecular Weight 352.4322
Wiswesser Line Notation 5VOR DNUNR DV2
Evaluation A
Smectic A-nematic; nematic-isotropic;
smectic A-smectic B (montropic phase) liquid
phase change data also given:
411.65 K, ΔH = 3933 J·mol^{-1};
420.65 K, ΔH = 879 J·mol^{-1};
361.65 K, ΔH = 2720 J·mol^{-1}.

$C_{21}H_{24}O_4$ (c) 87LES/LIC
2,2-Bis(phenyl-4-glycidoxy)propane
Heat Capacity 298 K, C_p = 485.9 J·mol^{-1}·K^{-1}
Temperature range 250 to 300 K.
Phase Changes
c/liq 313 K
Molecular Weight 340.4182
Wiswesser Line Notation T3OTJ B1OR DXR DO1- BT3OTJ
Evaluation B

$C_{21}H_{24}Si_3O_3$ (c) 81MEK/KAR
cis-Tri(methylphenyl)trisiloxane
Heat Capacity 298.15 K, C_p = 538.5 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Data given graphically.
Entropy 298.15 K, S = 571.1 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 373.2 K, ΔH = 47254 J·mol^{-1}
ΔS = 115.5 J·mol^{-1}·K^{-1}
Molecular Weight 408.6753
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 AR C1
CR E1 ER−C
Evaluation A

$C_{21}H_{24}Si_3O_3$ (c) 81MEK/KAR
trans-Tri(methylphenyl)trisiloxane
Heat Capacity 298.15 K, C_p = 506.7 J·mol^{-1}·K^{-1}
Temperature range 13 to 390 K.
Data given graphically.
Entropy 298.15 K, S = 564 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 320.9 K, ΔH = 43769 J·mol^{-1}
ΔS = 136.4 J·mol^{-1}·K^{-1}
Molecular Weight 408.6753
Wiswesser Line Notation T6-SI-O-SI-O-SI-OTJ A1 AR C1
CR E1 ER−T
Evaluation A

$C_{21}H_{25}N$ (c) 83MAR/THO
Octylcyanobiphenyl
Phase Changes
liq/liq ΔH = 0.4 J·mol^{-1}
Smectic A− nematic.
liq/liq ΔH = 612 J·mol^{-1}
Nematic− isotropic.
c/liq ΔH = 25700 J·mol^{-1}
Solid-smectic A.
Molecular Weight 291.4352
Wiswesser Line Notation NCR DR D8
Evaluation D

$C_{21}H_{25}N$ (liq) 82THO/MAR
Octylcyanobiphenyl
Phase Changes
c/liq 294.45 K, ΔH = 25700 J·mol^{-1}
ΔS = 87.3 J·mol^{-1}·K^{-1}
Solid-smectic A.
liq/liq 306.921 K
Smectic A-nematic.
Continuous transition with an upper limit of 0.4J·mol^{-1}.
liq/liq 313.91 K, ΔH = 612 J·mol^{-1}
ΔS = 1.95 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 291.4352
Wiswesser Line Notation NCR DR D8
Evaluation B

$C_{21}H_{25}NO_5$ (c) 82RAC/MAS
4-Nitrophenyl-4′-octyloxybenzoate
Heat Capacity 300 K, C_p = 510 J·mol^{-1}·K^{-1}
Temperature range 100 to 356 K.
Data given graphically.
Value given is an estimate from the graph.
Phase Changes
c/liq 323.70 K, ΔH = 34426 J·mol^{-1}
ΔS = 106.4 J·mol^{-1}·K^{-1}
Solid-smectic.
liq/liq 334.9 K, ΔH = 213 J·mol^{-1}
ΔS = 0.59 J·mol^{-1}·K^{-1}
Smectic-nematic.
liq/liq 341.2 K, ΔH = 448 J·mol^{-1}
ΔS = 1.3 J·mol^{-1}·K^{-1}
Nematic-isotropic.
Molecular Weight 371.4322
Wiswesser Line Notation WNR DOVR DO8
Evaluation B

$C_{21}H_{25}NO_5$ (c) 79BAT/BUK
4′-Nitrophenyl-4-*n*-octyloxybenzoate
Phase Changes
c,II/liq 323.2 K, ΔH = 34720 J·mol^{-1}
ΔS = 108 J·mol^{-1}·K^{-1}
liq/liq 334 K, ΔH = 90 J·mol^{-1}
ΔS = 0.30 J·mol^{-1}·K^{-1}
Smectic-A-nematic.
liq/liq 341 K, ΔH = 290 J·mol^{-1}
ΔS = 0.88 J·mol^{-1}·K^{-1}
Nematic-isotropic.
c,II/c,I 323 K
Molecular Weight 371.4322
Wiswesser Line Notation WNR DOVR DO8
Evaluation B

$C_{21}H_{44}$ (c) 55SCH/BUS
n-Henicosane
Phase Changes
c,II/c,I 305.65 K, ΔH = 15481 J·mol^{-1}
ΔS = 50.6 J·mol^{-1}·K^{-1}
c,I/liq 313.35 K, ΔH = 47698 J·mol^{-1}
ΔS = 152.2 J·mol^{-1}·K^{-1}
Molecular Weight 296.5786
Wiswesser Line Notation 21H
Evaluation B

$C_{22}H_{13}N_3O_7$ (c) 79FAR/SHA
Fluoranthene picric acid
Phase Changes
c,II/c,I 365.6 K, ΔH = 13800 J·mol^{-1}
ΔS = 37.7 J·mol^{-1}·K^{-1}
c/liq 462.4 K, ΔH = 24700 J·mol^{-1}
ΔS = 53.4 J·mol^{-1}·K^{-1}
Molecular Weight 431.3606
Wiswesser Line Notation L C6566 1A PJ &WNR BQ CNW ENW
Evaluation B

$C_{22}H_{13}N_3O_7$ (c) 79FAR/SHA
Pyrene picric acid
Phase Changes
c,III/c,II 443.2 K, ΔH = 2900 J·mol^{-1}
ΔS = 6.5 J·mol^{-1}·K^{-1}
c,II/c,I 456.6 K, ΔH = 1200 J·mol^{-1}
ΔS = 2.6 J·mol^{-1}·K^{-1}
c/liq 506.6 K, ΔH = 32600 J·mol^{-1}
ΔS = 64.4 J·mol^{-1}·K^{-1}
Molecular Weight 431.3606
Wiswesser Line Notation L666 B6 2AB PJ &WNR BQ CNW ENW
Evaluation B

$(C_{22}H_{14}N_2O_7)_n$ (c) 77KAR/BAZ
Poly-(p,p′-diphenylene oxide)pyromellitimide
Heat Capacity 300 K, C_p = 592.4 J·mol^{-1}·K^{-1}
Temperature range 60 to 400 K.
Entropy 300 K, ΔS = 543.9 J·mol^{-1}·K^{-1}
Molecular Weight 418.3619
Wiswesser Line Notation /*MVR BVQ DVQ EVMR DOR D*/
Evaluation B

$C_{22}H_{14}O_4$ (c) 77KAR/RAB
1,4-Bis(phenylglyoxaloyl)benzene
Heat Capacity 300 K, C_p = 435 J·mol^{-1}·K^{-1}
Temperature range 100 to 700 K.
Data given graphically.
Value estimated from graph.
Entropy 300 K, S = 381.0 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 425.1 K, ΔH = 32300 J·mol^{-1}
ΔS = 76.0 J·mol^{-1}·K^{-1}
Molecular Weight 342.3502
Wiswesser Line Notation RVVR DVVR
Evaluation C(C_p),A(S,Phase changes)

$C_{22}H_{18}N_4O_4$ (c) 79KAR/SAP
4′,4″-Diphenylenephthalidodicarboxylic acid dihydrazide
Heat Capacity 298.15 K, C_p = 460.7 J·mol^{-1}·K^{-1}
Temperature range 60 to 298 K.
Entropy 298.15 K, S = 441.4 J·mol^{-1}·K^{-1}
Molecular Weight 402.4086
Wiswesser Line Notation T56 BHOVT&J BR DVMZ& BR DVMZ
Evaluation A

$C_{22}H_{18}O_4$ (c) 84OZC/ASR
4,4′-Dipropanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 351 K, ΔH = 586 J·mol^{-1}
ΔS = 1.674 J·mol^{-1}·K^{-1}
c,II/c,I 359 K, ΔH = 7530 J·mol^{-1}
ΔS = 20.96 J·mol^{-1}·K^{-1}
c,I/liq 430 K, ΔH = 19400 J·mol^{-1}
ΔS = 45.35 J·mol^{-1}·K^{-1}
Solid-nematic.
Molecular Weight 346.3818
Wiswesser Line Notation 2VOR D1UU2UU1R DOV2
Evaluation A
Nematic-isotropic liquid phase change data also given:
470 K, ΔH = 1380 J·mol^{-1},
ΔS = 2.929 J·mol^{-1}·K^{-1}.

$C_{22}H_{20}N_2O_2$ (c) 87BYK/KIP
3-Phenyl-5-phenoxymethyl-2-N-phenyliminooxazolidine
Heat Capacity 298.15 K, C_p = 400.2 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 426.2 J·mol^{-1}·K^{-1}
Molecular Weight 344.4122
Wiswesser Line Notation T5NYOTJ AR BUNR D1OR
Evaluation A

$C_{22}H_{26}$ (c) 83KRA/BEC
1,1′-Diphenyl-1,1′-bicyclopentane
Heat Capacity 298 K, C_p = 375.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.309 Cal.K^{-1}.g^{-1}.
Molecular Weight 290.4474
Wiswesser Line Notation L5TJ AR A- AL5TJ AR
Evaluation B

$C_{22}H_{26}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-heptanoyloxyazobenzene
Phase Changes
c/liq 365.15 K, ΔH = 24811 J·mol^{-1}
ΔS = 67.95 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 366.4590
Wiswesser Line Notation 6VOR DNUNR DV2
Evaluation A
Smectic A-nematic; nematic-isotropic;
smectic A-montropic hexatic;
hexatic-montropic smectic B liquid phase change data also given:
414.65 K, ΔH = 5314 J·mol^{-1};
416.65 K , ΔH = 920 J·mol^{-1};
362.85 K, ΔH = 1590 J·mol^{-1};
358.55 K, ΔH = 84 J·mol^{-1}.

$C_{22}H_{27}N$ (c) 83MAR/THO
Nonylcyanobiphenyl
Phase Changes
liq/liq 320.8 K, ΔH = 5 J·mol^{-1}
ΔS = 0.02 J·mol^{-1}·K^{-1}
Smectic A— nematic.
liq/liq 322.7 K, ΔH = 1200 J·mol^{-1}
ΔS = 3.7 J·mol^{-1}·K^{-1}
Nematic— isotropic.
c/liq ΔH = 34500 J·mol^{-1}
Solid— smectic A.
Molecular Weight 305.4620
Wiswesser Line Notation NCR DR D9
Evaluation D

$C_{22}H_{28}N_2O_4Ni$ (c) 72ARA/SOR
Bis[N-(3-methoxysalicylidene)isopropylamine] nickel(II)
Heat Capacity 299.010 K, C_p = 741.87 J·mol^{-1}·K^{-1}
Temperature range 230 to 343 K.
Unsmoothed experimental datum.
Molecular Weight 443.1742
Wiswesser Line Notation T6 C6-NI- BO JNJ DO1 JY1&1 A-& AT6 C6-NI- BO JNJ DO1 JY1&1
Evaluation B
T(glass) = 297.5 K, ΔC_p = 172 J·mol^{-1}·K^{-1}.

$C_{22}H_{28}O_2$ (c) 79LEW/ENE
Northindrone acetate
Phase Changes
c/liq 480 K, ΔH = 27300 J·mol^{-1}; ΔS = 56.9 J·mol^{-1}·K^{-1}
Molecular Weight 324.4620
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FOV1
Evaluation A

$C_{22}H_{29}NO$ (c) 83SOR/TAN
N-*p*-*n*-Pentyloxybenzylidene-*p'*-*n*-butylaniline
Heat Capacity 298.15 K, C_p = 512.71 J·mol^{-1}·K^{-1}
Temperature range 11 to 393 K.
C_p = 2.3491T − 187.67 J·mol^{-1}·K^{-1} (11 to 299.69 K).
C_p value is calculated from equation.
Entropy 280 K, S = 478.16 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 299.69 K, ΔH = 22680 J·mol^{-1}; ΔS = 75.70 J·mol^{-1}·K^{-1}
Solid-smectic G liquid transition.
liq/liq 325.72 K, ΔH = 7110 J·mol^{-1}; ΔS = 21.79 J·mol^{-1}·K^{-1}
Smectic G− nematic liquid transition.
liq/liq 342.48 K, ΔH = 1780 J·mol^{-1}; ΔS = 5.22 J·mol^{-1}·K^{-1}
Nematic− isotropic liquid transition.
Molecular Weight 323.4772
Wiswesser Line Notation 5OR D1UNR D4
Evaluation A

$C_{22}H_{29}NO$ (gls) 83SOR/TAN
N-*p*-*n*-Pentyloxybenzylidene-*p'*-*n*-butylaniline
Heat Capacity 300 K, C_p = 561.46 J·mol^{-1}·K^{-1}
Temperature range 10 to 320 K.
Entropy 300 K, S = 588.03 J·mol^{-1}·K^{-1}
Molecular Weight 323.4772
Wiswesser Line Notation 5OR D1UNR D4
Evaluation A
Glassy and undercooled S_G phase.

$C_{22}H_{42}O_4$ (liq) 85OVC/MOS
Di(2-ethylhexyl)adipate
Heat Capacity 300 K, C_p = 701.5 J·mol^{-1}·K^{-1}
Temperature range 6 to 300 K.
Entropy 300 K, S = 865 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 161.5 K
Glass transition.
Molecular Weight 370.5714
Wiswesser Line Notation 4Y1&1OV4VO1Y1&4
Evaluation A

$C_{22}H_{42}O_4$ (liq) 75PHI/WAL
Di-*n*-hexyl sebacate
Heat Capacity 303.15 K, C_p = 711 J·mol^{-1}·K^{-1}
Temperature range 303 to 393 K.
Phase Changes
c/liq 274 K
Molecular Weight 370.5714
Wiswesser Line Notation 60V8VO6
Evaluation B

$C_{22}H_{44}$ (c) 69BOR/DAL
1,1,10,10-Tetramethylcyclooctadecane
Phase Changes
c/liq 359 K, ΔH = 39581 J·mol^{-1}; ΔS = 110 J·mol^{-1}·K^{-1}
Molecular Weight 308.5896
Wiswesser Line Notation L-18-TJ A1 A1 J1 J1
Evaluation B

$C_{22}H_{46}$ (c) 55SCH/BUS
n-Docosane
Phase Changes
c,II/c,I 316.15 K, ΔH = 28200 J·mol^{-1}; ΔS = 89.2 J·mol^{-1}·K^{-1}
c,I/liq 317.15 K, ΔH = 48953 J·mol^{-1}; ΔS = 154.4 J·mol^{-1}·K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 73COM
n-Docosane
Phase Changes
c,II/c,I 316.25 K, ΔH = 28200 J·mol^{-1}; ΔS = 89.2 J·mol^{-1}·K^{-1}
c,I/liq 317.25 K, ΔH = 48952 J·mol^{-1}; ΔS = 154.3 J·mol^{-1}·K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 79CLA/LET
n-Docosane
Phase Changes
c,II/c,I 315.15 K, ΔH = 29505 J·mol^{-1}; ΔS = 93.6 J·mol^{-1}·K^{-1}
c,I/liq 316.05 K, ΔH = 47837 J·mol^{-1}; ΔS = 151.4 J·mol^{-1}·K^{-1}
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{22}H_{46}$ (c) 81HOE
n-Docosane
Heat Capacity 300 K, C_p = 468 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K. C_v = 1.48 J·g^{-1}·K^{-1}.
Molecular Weight 310.6054
Wiswesser Line Notation 22H
Evaluation B

$C_{23}H_{15}N_3O_7$ (c) 79FAR/SHA
1,2-Benzfluorene picric acid
Phase Changes
c/liq 402.7 K, ΔH = 45600 J·mol^{-1}; ΔS = 113.2 J·mol^{-1}·K^{-1}
Molecular Weight 445.3874
Wiswesser Line Notation L D6 B566 CHJ &WNR BQ CNW ENW
Evaluation B

$C_{23}H_{15}N_3O_7$ (c) 79FAR/SHA
2,3-Benzfluorene picric acid
Phase Changes
c/liq 392.8 K, ΔH = 33500 J·mol^{-1}
ΔS = 85.3 J·mol^{-1}·K^{-1}
Molecular Weight 445.3874
Wiswesser Line Notation L D6 B656 LHJ &WNR BQ CNW ENW
Evaluation B

$C_{23}H_{17}N$ (c) 85LEB/BYK
2,4,6-Triphenylpyridine
Heat Capacity 298.15 K, C_p = 358.6 J·mol^{-1}·K^{-1}
Temperature range 5 to 330 K.
Entropy 298.15 K, S = 371.6 J·mol^{-1}·K^{-1}
Molecular Weight 307.3940
Wiswesser Line Notation T6NJ BR DR FR
Evaluation A

$C_{23}H_{17}N$ (c) 84BYK/KIP
2,4,6-Triphenylpyridine
Heat Capacity 298.15 K, C_p = 358.6 J·mol^{-1}·K^{-1}
Temperature range 14 to 330 K.
Entropy 298.15 K, S = 371.6 J·mol^{-1}·K^{-1}
Molecular Weight 307.3940
Wiswesser Line Notation T6NJ BR DR FR
Evaluation A

$C_{23}H_{28}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-octanoyloxyazobenzene
Phase Changes
c/liq 369.65 K, ΔH = 27489 J·mol^{-1}
ΔS = 74.36 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 380.4858
Wiswesser Line Notation 7VOR DNUNR DV2
Evaluation A
Smectic A-nematic; nematic-isotropic; smectic A-monotropic hexatic; hexatic-monotropic smectic B liquid phase change data also given:
416.15 K, ΔH = 5314 J·mol^{-1};
416.65 K, ΔH = 1004 J·mol^{-1};
359.85 K, ΔH = 1423 J·mol^{-1};
353.75 K, ΔH = 42 J·mol^{-1}.

$C_{23}H_{29}N$ (c) 83MAR/THO
Decylcyanobiphenyl
Phase Changes
liq/liq ΔH = 2830 J·mol^{-1}
Smectic A– isotropic.
c/liq ΔH = 36000 J·mol^{-1}
Solid– smectic A.
Molecular Weight 319.4888
Wiswesser Line Notation NCR DR D10
Evaluation D

$C_{23}H_{31}NO$ (c) 83YOS/SOR3
N-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline
Heat Capacity 298.15 K, C_p = 512.02 J·mol^{-1}·K^{-1}
Temperature range 11 to 393 K.
Entropy 298.15 K, S = 537.57 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 306.60 K, ΔH = 23290 J·mol^{-1}
ΔS = 75.98 J·mol^{-1}·K^{-1}
Solid-smectic G.
Molecular Weight 337.5040
Wiswesser Line Notation 60*R* D1UNR D4
Evaluation A
Smectic G-smectic B; smectic B-smectic A; smectic A-nematic; nematic-isotropic liquid phase change data given:
331.56 K, ΔH = 804 J·mol^{-1}, ΔS = 2.53 J·mol^{-1}·K^{-1};
332.86 K, ΔH = 3370 J·mol^{-1}, ΔS = 10.14 J·mol^{-1}·K^{-1};
343.24 K, ΔH = 3200 J·mol^{-1}, ΔS = 9.37 J·mol^{-1}·K^{-1};
350.92 K, ΔH = 1890 J·mol^{-1}, ΔS = 5.37 J·mol^{-1}·K^{-1}.

$C_{23}H_{31}NO$ (gls) 83YOS/SOR3
N-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline
Heat Capacity 300 K, C_p = 595.14 J·mol^{-1}·K^{-1}
Temperature range 10 to 310 K.
Entropy 300 K, S = 615.04 J·mol^{-1}·K^{-1}
Residual entropy of the glassy state at 0 K was estimated to be 7.51 ± 0.63 J·mol^{-1}·K^{-1}.
Molecular Weight 337.5040
Wiswesser Line Notation 6OR D1UNR D4
Evaluation A

$C_{23}H_{48}$ (c) 84SYU/TUM
Tricosane
Phase Changes
c/liq 319.7 K, ΔH = 76700 J·mol^{-1}
ΔS = 239.9 J·mol^{-1}·K^{-1}
Relative error in determination ± 5%.
Molecular Weight 324.6322
Wiswesser Line Notation 23H
Evaluation C

$C_{23}H_{48}$ (c) 55SCH/BUS
n-Tricosane
Phase Changes
c,II/c,I 313.65 K, ΔH = 21757 J·mol^{-1}
ΔS = 69.4 J·mol^{-1}·K^{-1}
c,I/liq 320.65 K, ΔH = 53974 J·mol^{-1}
ΔS = 168.3 J·mol^{-1}·K^{-1}
Molecular Weight 324.6322
Wiswesser Line Notation 23H
Evaluation B

$(C_{24}H_{12}N_6)_n$ (c) 88LEB/BYK
Polytriazine
Heat Capacity 298.15 K, C_p = 395.3 J·mol^{-1}·K^{-1}
Temperature range 0 to 330 K.
Entropy 298.15 K, S = 451.6 J·mol^{-1}·K^{-1}
Molecular Weight 384.3990
Wiswesser Line Notation /T6N CN ENJ BR DYUN*&* DR DYUN*&* FR DYUN*&*/ 1/3
Evaluation A

$C_{24}H_{15}N_3O_7$ (c) 79FAR/SHA
Triphenylene picric acid
Phase Changes
c/liq 501.4 K, ΔH = 46900 J·mol^{-1}
ΔS = 93.6 J·mol^{-1}·K^{-1}
Molecular Weight 457.3984
Wiswesser Line Notation L B6 H666J &WNR BQ CNW ENW
Evaluation B

$C_{24}H_{15}N_3O_7$ (c) 79FAR/SHA
1,2-Benzanthracene picric acid
Phase Changes
c/liq 414.3 K, ΔH = 32200 J·mol^{-1}
ΔS = 77.7 J·mol^{-1}·K^{-1}
Molecular Weight 457.3984
Wiswesser Line Notation L D6 C666J &WNR BQ CNW ENW
Evaluation B

$C_{24}H_{18}$ (c) 82LEB/BYK
1,3,5-Triphenylbenzene
Heat Capacity 298.15 K, C_p = 361.0 J·mol^{-1}·K^{-1}
Temperature range 13.8 to 480 K.
Entropy 298.15 K, S = 375.5 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 446 K, ΔH = 33400 J·mol^{-1}
ΔS = 75.1 J·mol^{-1}·K^{-1}
Molecular Weight 306.4063
Wiswesser Line Notation RR CR ER
Evaluation A

$C_{24}H_{18}$ (c) 79SMI
p-Quaterphenyl
Phase Changes
c/liq 587.2 K, ΔH = 37800 J·mol^{-1}
ΔS = 64.4 J·mol^{-1}·K^{-1}
Molecular Weight 306.4062
Wiswesser Line Notation RR DR DR
Evaluation A

$C_{24}H_{18}$ (c) 82WAS/RAD
p-Quaterphenyl
Heat Capacity 300 K, C_p = 340 J·mol^{-1}·K^{-1}
Temperature range 180 to 600 K.
Data given graphically.
Value estimated from graph.
Phase Changes
c,III/c,II 190–260 K, ΔH = 1100 J·mol^{-1}
c,II/c,I 450–540 K, ΔH = 1000 J·mol^{-1}
c/liq 586.7 K, ΔH = 57600 J·mol^{-1}
ΔS = 98.2 J·mol^{-1}·K^{-1}
Molecular Weight 306.4062
Wiswesser Line Notation RR DR DR
Evaluation C(C_p), B(Phase changes)

$C_{24}H_{18}$ (c) 85SAI/ATA
p-Quaterphenyl
Heat Capacity 298.15 K, C_p = 362.52 J·mol^{-1}·K^{-1}
Temperature range 3 to 300 K.
Entropy 298.15 K, S = 363.64 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 233.0 K, ΔH = 414 J·mol^{-1}
ΔS = 1.82 J·mol^{-1}·K^{-1}
Transition region 180 to 270 K.
Molecular Weight 306.4062
Wiswesser Line Notation RR DR DR
Evaluation A

$C_{24}H_{20}BK$ (c) 57DAV/STA
Potassium tetraphenyl boron
Heat Capacity 298.15 K, C_p = 418.23 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 440.16 J·mol^{-1}·K^{-1}
Molecular Weight 358.3303
Wiswesser Line Notation RBR&R&R &-KA-
Evaluation B

$C_{24}H_{20}BRb$ (c) 57DAV/STA
Rubidium tetraphenyl boron
Heat Capacity 298.15 K, C_p = 412.96 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 444.76 J·mol^{-1}·K^{-1}
Molecular Weight 404.6998
Wiswesser Line Notation RBR&R&R &-RB-
Evaluation B

$C_{24}H_{20}CrI$ (c) 72NIK/SAF
Bis(biphenyl)chromium iodide
Heat Capacity 298.15 K, C_p = 437.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 298.15 K.
Entropy 298.15 K, S = 424.7 J·mol^{-1}·K^{-1}
Molecular Weight 487.3225
Wiswesser Line Notation L6ØJA- AL6ØJ Ø-CR--ØL6ØJA- AL6ØJ &I
Evaluation B

$C_{24}H_{22}O_4$ (c) 84OZC/ASR
4,4′-Dibutanoyloxydiphenyldiacetylene
Phase Changes
c,V/c,IV 319 K, ΔH = 10400 J·mol^{-1}
ΔS = 32.51 J·mol^{-1}·K^{-1}
c,IV/c,III 368 K, ΔH = 1510 J·mol^{-1}
ΔS = 4.100 J·mol^{-1}·K^{-1}
c,III/c,II 400 K
c,II/c,I 408 K, ΔH = 12.5 J·mol^{-1}
ΔS = 0.2929 J·mol^{-1}·K^{-1}
c,II/c,II,c,II/c,I transitions combined.
c,I/liq 416 K, ΔH = 20100 J·mol^{-1}
ΔS = 48.28 J·mol^{-1}·K^{-1}
Solid-nematic.
Molecular Weight 374.4354
Wiswesser Line Notation 3VOR D1UU2UU1R DOV3
Evaluation A
Nematic-isotropic liquid phase change data also given:
453 K, ΔH = 1250 J·mol^{-1},
ΔS = 2.76 J·mol^{-1}·K^{-1}.

$C_{24}H_{24}BN$ (c) 57DAV/STA
Ammonium tetraphenyl boron
Heat Capacity 298.15 K, C_p = 434.93 J·mol^{-1}·K^{-1}
Temperature range 20 to 298 K.
Entropy 298.15 K, S = 457.31 J·mol^{-1}·K^{-1}
Molecular Weight 337.2703
Wiswesser Line Notation RBR&R&R &ZH
Evaluation B

$C_{24}H_{28}O_2Si_3$ (liq) 81SHA/DZH
1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane
Heat Capacity 298 K, C_p = 648 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Entropy 298 K, S = 769 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 270.49 K, ΔH = 22753 J·mol^{-1}
ΔS = 84.12 J·mol^{-1}·K^{-1}
Molecular Weight 432.7405
Wiswesser Line Notation 1-SI-1&1&O-SI-R&R&O-SI-1&1&1
Evaluation A
T(glass) = 178 K.

$C_{24}H_{30}$ (c) 83KRA/BEC
1,1′-Diphenyl-1,1′-bicyclohexane
Heat Capacity 298 K, C_p = 403.8 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.303 Cal.K^{-1}.g^{-1}.
Molecular Weight 318.5010
Wiswesser Line Notation L6TJ AR A- AL6TJ AR
Evaluation B

$C_{24}H_{30}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-nonanoyloxyazobenzene
Phase Changes
c/liq 367.15 K, ΔH = 3017 J·mol^{-1}
ΔS = 8.22 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 394.5126
Wiswesser Line Notation 8VOR DNUNR DV2
Evaluation A
Smectic A-isotropic; smectic A-monotropic hexatic;
hexatic-monotropic smectic B liquid phase change data also given:
417.15 K, ΔH = 7029 J·mol^{-1};
361.05 K, ΔH = 1757J·mol^{-1};
353.25 K, ΔH = 42 J·mol^{-1}.

$C_{24}H_{31}N$ (c) 83MAR/THO
Undecylcyanobiphenyl
Phase Changes
liq/liq ΔH = 3800 J·mol^{-1}
Smectic A— isotropic.
c/liq ΔH = 43200 J·mol^{-1}
Solid— smectic A.
Molecular Weight 333.5156
Wiswesser Line Notation NCR NR D11
Evaluation D

$C_{24}H_{32}O_3$ (liq) 85SHA/ZHU
4-*n*-Heptoxyphenyl-4'-*n*-butylbenzoate
Heat Capacity 312.14 K, C_p = 793.4 J·mol^{-1}·K^{-1}
Temperature range 312 to 354 K.
Unsmoothed experimental datum.
Phase Changes
liq/liq 317.3 K, ΔH = 490 J·mol^{-1}
ΔS = 1.54 J·mol^{-1}·K^{-1}
Molecular Weight 368.5150
Wiswesser Line Notation 7OR DOVR D4
Evaluation B

$C_{24}H_{34}$ (liq) 60KAR/STR4
1,1-Diphenyldodecane
Heat Capacity 298.15 K, C_p = 593.9 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 684.9 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 191 K, ΔH = 1928 J·mol^{-1}
ΔS = 10.1 J·mol^{-1}·K^{-1}
c,I/liq 281.40 K, ΔH = 38844 J·mol^{-1}
ΔS = 138.1 J·mol^{-1}·K^{-1}
Molecular Weight 322.5326
Wiswesser Line Notation 11YR&R
Evaluation A
See also 60KAR/STR2.

$C_{24}H_{38}O_4$ (c) 70MAR/RAB
Di-(2-ethylhexyl) *o*-phthalate
Molecular Weight 390.5618
Wiswesser Line Notation 4Y2&1OVR BVO1Y2&4
Evaluation B
T(glass) = 182.5 °C.

$C_{24}H_{38}O_4$ (liq) 85RAB/NOV
Di-(2-ethylhexyl) *o*-phthalate
Heat Capacity 298.15 K, C_p = 704.7 J·mol^{-1}·K^{-1}
Temperature range 14 to 300 K.
Entropy 298.15 K, S = 807.7 J·mol^{-1}·K^{-1}
Molecular Weight 390.5618
Wiswesser Line Notation 4Y2&1OVR BVO1Y2&4
Evaluation A
Data given for glassy state from 10 to 180 K.
Glass transition temperature,
T(glass)= 182.5 K.

$C_{24}H_{38}O_4$ (c) 70MAR/RAB
Dioctyl *o*-phthalate
Heat Capacity 300 K, C_p = 707.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 360 K.
Entropy 300 K, S = 755.2 J·mol^{-1}·K^{-1}
Molecular Weight 390.5618
Wiswesser Line Notation 80VR BVO8
Evaluation B

$C_{24}H_{40}$ (liq) 60KAR/STR4
1-Phenyl-1-cyclohexyldodecane
Heat Capacity 298.15 K, C_p = 611.1 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 695.9 J·mol^{-1}·K^{-1}
Phase Changes
c,I/liq 275.84 K, ΔH = 35171 J·mol^{-1}
ΔS = 127.7 J·mol^{-1}·K^{-1}
Molecular Weight 328.5800
Wiswesser Line Notation L6TJ AY11&R
Evaluation A

$C_{24}H_{46}$ (c) 60KAR/STR4
1,1-Dicyclohexyldodecane
Heat Capacity 298.15 K, C_p = 562.6 J·mol^{-1}·K^{-1}
Temperature range 10 to 300 K.
Entropy 298.15 K, S = 545.7 J·mol^{-1}·K^{-1}
Phase Changes
c/liq 300.58 K, ΔH = 44267 J·mol^{-1}
ΔS = 147.3 J·mol^{-1}·K^{-1}
Molecular Weight 334.6274
Wiswesser Line Notation L6TJ AY11&- AL6TJ
Evaluation A

$C_{24}H_{50}$ (c) 55SCH/BUS
n-Tetracosane
Phase Changes
c,II/c,I 321.25 K, ΔH = 31296 J·mol^{-1}
ΔS = 97.4 J·mol^{-1}·K^{-1}
c,I/liq 323.75 K, ΔH = 54894 J·mol^{-1}
ΔS = 169.5 J·mol^{-1}·K^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (c) 73COM
n-Tetracosane
Phase Changes
c,II/c,I 321.35 K, ΔH = 31296 J·mol^{-1}
ΔS = 97.4 J·mol^{-1}·K^{-1}
c,I/liq 323.85 K, ΔH = 54894 J·mol^{-1}
ΔS = 169.6 J·mol^{-1}·K^{-1}
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (c) 81HOE
n-Tetracosane
Heat Capacity 300 K, C_p = 601 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K.
Cv = 1.75 J·g^{-1}·K^{-1}.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation B

$C_{24}H_{50}$ (c) 84SYU/TUM
n-Tetracosane
Phase Changes
c/liq 322.0 K, ΔH = 81750 J·mol^{-1}
ΔS = 253.9 J·mol^{-1}·K^{-1}
Relative error in determination ± 5%.
Molecular Weight 338.6590
Wiswesser Line Notation 24H
Evaluation C

$C_{24}H_{56}Cl_4MnN_2$ (c) 87ZHA
Dodecylammonium tetrachloromanganate (II)
Heat Capacity 298.15 K, C_p = 869.8 J·mol^{-1}·K^{-1}
Temperature range 280 to 500 K.
Phase Changes
c,III/c,II 330.6 K, ΔH = 47780 J·mol^{-1}
ΔS = 144.5 J·mol^{-1}·K^{-1}
c,II/c,I 334.5 K, ΔH = 5960 J·mol^{-1}
ΔS = 17.82 J·mol^{-1}·K^{-1}
Molecular Weight 569.4698
Wiswesser Line Notation -12-ZH 2 .MN G4
Evaluation A

$C_{24}H_{56}Cl_4MnN_2$ (c) 88ZHA/YAN
Dodecylammonium tetrachloromanganate (II)
Heat Capacity 298.15 K, C_p = 869.8 J·mol^{-1}·K^{-1}
Temperature range 280 to 500 K.
Phase Changes
c,III/c,II 330.6 K, ΔH = 47780 J·mol^{-1}
ΔS = 144.5 J·mol^{-1}·K^{-1}
c,II/c,I 334.5 K, ΔH = 5960 J·mol^{-1}
ΔS = 17.82 J·mol^{-1}·K^{-1}
Molecular Weight 569.4698
Wiswesser Line Notation -12-ZH 2 .MN G4
Evaluation A

$C_{24}H_{56}Cl_4N_2Zn$ (c) 88ZHA/YAN
Dodecylammonium tetrachlorozincate (II)
Heat Capacity 298.15 K, C_p = 851.7 J·mol^{-1}·K^{-1}
Temperature range 280 to 500 K.
Phase Changes
c,II/c,I 364.3 K, ΔH = 66790 J·mol^{-1}
ΔS = 183.3 J·mol^{-1}·K^{-1}
c,I/liq 435.1 K, ΔH = 9120 J·mol^{-1}
ΔS = 20.96 J·mol^{-1}·K^{-1}
Molecular Weight 579.9118
Wiswesser Line Notation -12-ZH 2 .ZN G4
Evaluation A

$C_{24}H_{56}Cl_4N_2Zn$ (c) 88ZHA/YAN
Dodecylammonium tetrachlorozincate (II)
Heat Capacity 298.15 K, C_p = 851.7 J·mol^{-1}·K^{-1}
Temperature range 280 to 500 K.
Phase Changes
c,II/c,I 364.3 K, ΔH = 66790 J·mol^{-1}
ΔS = 183.3 J·mol^{-1}·K^{-1}
c,I/liq 435.1 K, ΔH = 9120 J·mol^{-1}
ΔS = 20.96 J·mol^{-1}·K^{-1}
Molecular Weight 579.9118
Wiswesser Line Notation -12-Z 2 &GH 2 &-ZN- G2
Evaluation A

$C_{25}H_{32}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-decanoyloxyazobenzene
Phase Changes
c/liq 371.15 K, ΔH = 32928 J·mol^{-1}
ΔS = 88.72 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 408.5394
Wiswesser Line Notation 9VOR DNUNR DV2
Evaluation A
Smectic A-esotropic; smectic A-monotropic
hexatic liquid phase change data also given:
417.65 K, ΔH = 7196 J·mol^{-1};
359.95 K, ΔH = 1088 J·mol^{-1}.

$C_{25}H_{34}O_2$ (c) 79LEW/ENE
Northindrone dimethylpropionate
Phase Changes
c/liq 500 K, ΔH = 37800 J·mol^{-1}
ΔS = 75.6 J·mol^{-1}·K^{-1}
Molecular Weight 366.5424
Wiswesser Line Notation L E5 B666 OV MUTJ E1
FOVX1&1&1 F1UU1
Evaluation A

$C_{25}H_{40}O_2Si_2$ (c) 79LEW/ENE
Northindrone pentamethyldisiloxyl ether
Phase Changes
c/liq 355 K, ΔH = 22900 J·mol^{-1}
ΔS = 64.5 J·mol^{-1}·K^{-1}
Molecular Weight 428.7608
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1
FO-SI-1&1&O-SI-1&1&1
Evaluation A

$C_{25}H_{48}O_4$ (liq) 83BAB/RAB
Bis(2-ethylhexyl)azelaate; Bis(2-ethylhexyl) nonadioate
Heat Capacity 298.15 K, C_p = 799.7 J·mol^{-1}·K^{-1}
Temperature range 13 to 335 K.
Entropy 298.15 K, S = 899.5 J·mol^{-1}·K^{-1}
Phase Changes
c,gls/liq 160.0 K
Molecular Weight 412.6518
Wiswesser Line Notation 4Y2&1OV7VO1Y2&4
Evaluation A

$C_{25}H_{52}$ (c) 55SCH/BUS
n-Pentacosane
Phase Changes
c,II/c,I 320.15 K, ΔH = 26066 J·mol^{-1}
ΔS = 81.4 J·mol^{-1}·K^{-1}
c,I/liq 326.65 K, ΔH = 57739 J·mol^{-1}
ΔS = 176.8 J·mol^{-1}·K^{-1}
Molecular Weight 352.6858
Wiswesser Line Notation 25H
Evaluation B

$C_{25}H_{52}$ (c) 79CLA/LET
n-Pentacosane
Phase Changes
c,II/c,I 319.85 K, ΔH = 25235 J·mol^{-1}
ΔS = 78.9 J·mol^{-1}·K^{-1}
c,I/liq 326.25 K, ΔH = 56605 J·mol^{-1}
ΔS = 173.5 J·mol^{-1}·K^{-1}
Molecular Weight 352.6858
Wiswesser Line Notation 25H
Evaluation B

$C_{26}H_{15}N_3O_7$ (c) 79FAR/SHA
Perylene picric acid
Phase Changes
c/liq 495.0 K, ΔH = 42300 J·mol^{-1}
ΔS = 85.5 J·mol^{-1}·K^{-1}
Molecular Weight 481.4204
Wiswesser Line Notation L666 L6 K6 2AL TJ &WNR BQ CNW ENW
Evaluation B

$C_{26}H_{15}N_3O_7$ (c) 79FAR/SHA
Benzo[a]pyrene picric acid
Phase Changes
c/liq 475.5 K, ΔH = 39300 J·mol^{-1}
ΔS = 82.7 J·mol^{-1}·K^{-1}
Molecular Weight 481.4204
Wiswesser Line Notation L D6 B6666 2AB TJ &WNR BQ CNW ENW
Evaluation B

$C_{26}H_{17}N_3O_7$ (c) 79FAR/SHA
β,β'-Binaphthyl picric acid
Phase Changes
c/liq 464.2 K, ΔH = 41400 J·mol^{-1}
ΔS = 89.2 J·mol^{-1}·K^{-1}
Molecular Weight 483.4362
Wiswesser Line Notation L66J A- AL66J &WNR BQ CNW ENW
Evaluation B

$C_{26}H_{20}N_6O$ (c) 84KAR/SHV
Bis-(o-aminophenyl)-2,2′-dibenzimidazole oxide
Heat Capacity 298.15 K, C_p = 471.1 J·mol^{-1}·K^{-1}
Temperature range 60 to 298 K.
Entropy 298.15 K, S = 426.3 J·mol^{-1}·K^{-1}
Molecular Weight 432.4838
Wiswesser Line Notation ZR B- CT56 BM DNJ H- 2 O
Evaluation B

$C_{26}H_{20}Sn$ (c) 85CAR/LAY
Triphenyl phenylethynyl tin
Heat Capacity 298.15 K, C_p = 447.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.992 J·K^{-1}·g^{-1}.
Molecular Weight 451.1340
Wiswesser Line Notation R-SN-R&R&1UU1R
Evaluation B

$C_{26}H_{26}O_4$ (c) 84OZC/ASR
4,4′-Dipentanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 272 K
c,II/c,I 290 K, ΔH = 1240 J·mol^{-1}
ΔS = 4.309 J·mol^{-1}·K^{-1}
c,II/c,II, c,II/c,I transitions combined.
c,I/liq 405 K, ΔH = 24700 J·mol^{-1}
ΔS = 61.04 J·mol^{-1}·K^{-1}
Solid-nematic.
Molecular Weight 402.4891
Wiswesser Line Notation 4VOR D1UU2UU1R DOV4
Evaluation A
Nematic-isotropic liquid phase change data also given:
434 K, ΔH = 2300 J·mol^{-1},
ΔS = 3.390 J·mol^{-1}·K^{-1}.

$C_{26}H_{34}$ (c) 83KRA/BEC
1,1′-Diphenyl-1,1′-bicyclooctane
Heat Capacity 298 K, C_p = 453.8 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.313 Cal.K^{-1}.g^{-1}.
Molecular Weight 346.5546
Wiswesser Line Notation L8TJ A*R* A- AL8TJ AR
Evaluation B

$C_{26}H_{34}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-undecanoyloxyazobenzene
Phase Changes
c/liq 370.65 K, ΔH = 37489 J·mol^{-1}
ΔS = 101.1 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 422.5662
Wiswesser Line Notation 10VOR DNUNR DV2
Evaluation A
Smectic A-isotropic liquid phase change data also given:
416.65 K, ΔH = 7573 J·mol^{-1}.

$C_{26}H_{38}$ (c) 83KRA/BEC
2,3-Dimethyl-2,3-bis(4-*tert*-butylphenyl)butane
Heat Capacity 298 K, C_p = 529.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.361 cal·K^{-1}·g^{-1}.
Molecular Weight 350.5862
Wiswesser Line Notation 1XR&R DX1&1&1 &X1&1&R DX1&1&1
Evaluation B

$C_{26}H_{52}$ (c) 69BOR/DAL

1,1,4,4,10,10,13,13-Octamethyl cyclooctadecane

Phase Changes

c,II/c,I	427 K,	ΔH = 6736 J·mol^{-1}
		ΔS = 15.9 J·mol^{-1}·K^{-1}
c/liq	438 K,	ΔH = 20167 J·mol^{-1}
		ΔS = 46.4 J·mol^{-1}·K^{-1}

Molecular Weight 364.6968
Wiswesser Line Notation L-18-TJ A1 A1 D1 D1 J1 J1 M1 M1
Evaluation B

$C_{26}H_{54}$ (c) 55SCH/BUS

n-Hexacosane

Phase Changes

c,II/c,I	326.45 K,	ΔH = 32217 J·mol^{-1}
		ΔS = 98.7 J·mol^{-1}·K^{-1}
c,I/liq	329.45 K,	ΔH = 59496 J·mol^{-1}
		ΔS = 180.6 J·mol^{-1}·K^{-1}

Molecular Weight 366.7126
Wiswesser Line Notation 26H
Evaluation B

$C_{26}H_{54}$ (c) 73COM

n-Hexacosane

Phase Changes

c,II/c,I	326.55 K,	ΔH = 34225 J·mol^{-1}
		ΔS = 104.8 J·mol^{-1}·K^{-1}
c,I/liq	329.55 K,	ΔH = 59496 J·mol^{-1}
		ΔS = 180.5 J·mol^{-1}·K^{-1}

Molecular Weight 366.7126
Wiswesser Line Notation 26H
Evaluation B

$C_{27}H_{30}O_2$ (c) 79LEW/ENE

Northindrone benzoate

Phase Changes

c/liq	531 K,	ΔH = 41500 J·mol^{-1}
		ΔS = 78.2 J·mol^{-1}·K^{-1}

Molecular Weight 386.5328
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FOVR
Evaluation A

$C_{27}H_{36}N_2O_3$ (c) 83FAN/POE

4-Propionyl-4′-*n*-dodecanoyloxyazobenzene

Phase Changes

c/liq	373.65 K,	ΔH = 38074 J·mol^{-1}
		ΔS = 101.9 J·mol^{-1}·K^{-1}

Solid-smectic A.
Molecular Weight 436.5930
Wiswesser Line Notation 11VOR DNUNR DV2
Evaluation A
Smectic A-isotropic liquid phase change data also given:
416.15 K, ΔH = 7866 J·mol^{-1}.

$C_{27}H_{38}O_2$ (c) 79LEW/ENE

Northindrone heptanoate

Phase Changes

c/liq	340 K,	ΔH = 21600 J·mol^{-1}
		ΔS = 63.5 J·mol^{-1}·K^{-1}

Molecular Weight 394.5960
Wiswesser Line Notation L E5 B666 OV MUTJ E1 FOV6 F1UU1
Evaluation A

$C_{27}H_{56}$ (c) 55SCH/BUS

n-Heptacosane

Phase Changes

c,II/c,I	320.25 K,	ΔH = 28953 J·mol^{-1}
		ΔS = 90.4 J·mol^{-1}·K^{-1}
c,I/liq	331.95 K,	ΔH = 60417 J·mol^{-1}
		ΔS = 182.0 J·mol^{-1}·K^{-1}

Molecular Weight 380.7394
Wiswesser Line Notation 27H
Evaluation B

$C_{28}H_{15}N_3O_7$ (c) 79FAR/SHA

o-Phenylenepyrene picric acid

Phase Changes

c/liq	469.6 K,	ΔH = 39300 J·mol^{-1}
		ΔS = 83.7 J·mol^{-1}·K^{-1}

Molecular Weight 505.4424
Wiswesser Line Notation L E6 D4 B6666 2AB TJ &WNR BQ CNW ENW WNR BQ CNW ENW
Evaluation B

$C_{28}H_{17}N_3O_7$ (c) 79FAR/SHA

Picene picric acid

Phase Changes

c,II/c,I	391 K,	ΔH = 3300 J·mol^{-1}
		ΔS = 8.4 J·mol^{-1}·K^{-1}
c/liq	437.9 K,	ΔH = 21300 J·mol^{-1}
		ΔS = 48.6 J·mol^{-1}·K^{-1}

Molecular Weight 507.4582
Wiswesser Line Notation L F6 E6 B666J &WNR BQ CNW ENW
Evaluation B

$C_{28}H_{17}N_3O_7$ (c) 79FAR/SHA

1,2,3,4-Dibenzanthracene picric acid

Phase Changes

c,II/c,I	446.5 K,	ΔH = 6700 J·mol^{-1}
		ΔS = 15.0 J·mol^{-1}·K^{-1}
c/liq	485.2 K,	ΔH = 44800 J·mol^{-1}
		ΔS = 92.3 J·mol^{-1}·K^{-1}

Molecular Weight 507.4582
Wiswesser Line Notation L D6 J6 C666J &WNR BQ CNW ENW
Evaluation B

$C_{28}H_{17}N_3O_7$ (c) 79FAR/SHA

1,2,5,6-Dibenzanthracene picric acid

Phase Changes

c/liq	493.0 K,	ΔH = 54000 J·mol^{-1}
		ΔS = 109.6 J·mol^{-1}·K^{-1}

Molecular Weight 507.4582
Wiswesser Line Notation L G6 D6 B666J &WNR BQ CNW ENW
Evaluation B

$C_{28}H_{18}N_6$ (c) 84RAB/KAR

Phthalonitrile and *m*-phenylene diamine condensation product

Heat Capacity 298.15 K, C_p = 446.5 J·mol^{-1}·K^{-1}
Temperature range 60 to 530 K.
Entropy 298.15 K, S = 424.3 J·mol^{-1}·K^{-1}
Molecular Weight 438.4904
Wiswesser Line Notation ZR CZ &NCR DCN
Evaluation A

$(C_{28}H_{24}GeSi)_n$ (gls) 78LEB/LEB2

Diphenylsilane — diethynyldi-phenylgermane vitreous copolymer; Polyvinlenediphenylsilyl,germyl-α,ω-dihydride copolymer

Heat Capacity 298.15 K C_p = 566.6 J·mol^{-1}·K^{-1}

Temperature range for devitrification 280 to 310 K

T(glass) = 301 K

Molecular Weight 461.1931

Wiswesser Line Notation /*-SI-R7R&1U1-GE-R&R&1U1*/

Evaluation A

Average molecular weight, n = 10,000

$(C_{28}H_{24}GeSi)_n$ (gls) 78LEB/RAB

Polyvinylenediphenylenesilyl,germyl-α,ω-dihydride copolymer

Heat Capacity 298.15 K, C_p = 566.6 J·mol^{-1}·K^{-1}

Temperature range 7 to 330 K.

Entropy 298.15 K, S = 583.8 J·mol^{-1}·K^{-1}

Glass like state.

Molecular Weight 461.1931

Wiswesser Line Notation /*-SI-R&R&1U1-GE-R&R&1U1*/

Evaluation A

T(glass) = 301 K.

$C_{28}H_{30}O_4$ (c) 84OZC/ASR

4,4′-Dihexanoyloxydiphenyldiacetylene

Phase Changes

c,III/c,II	343 K,	ΔH = 19000 J·mol^{-1}
		ΔS = 55.40 J·mol^{-1}·K^{-1}
c,II/c,I	396 K,	ΔH = 1460 J·mol^{-1}
		ΔS = 3.682 J·mol^{-1}·K^{-1}
c,I/liq	407 K,	ΔH = 26300 J·mol^{-1}
		ΔS = 64.64 J·mol^{-1}·K^{-1}

Solid-nematic.

Molecular Weight 430.5426

Wiswesser Line Notation 5VOR D1UU2UU1R DOV5

Evaluation A

Nematic-isotropic liquid phase change data also given:

430 K, ΔH = 1710 J·mol^{-1}, ΔS = 3.975 J·mol^{-1}·K^{-1}.

$C_{28}H_{32}Cl_4N_2Zn$ (c) 82FER/SOC

Bis-(tetradecylammonium)zinc tetrachloride

Heat Capacity

Temperature range 360 to 370 K.

Data given graphically.

Phase Changes

c,III/c,II	362.5 K,	ΔH = 9700 J·mol^{-1}
		ΔS = 22.5 J·mol^{-1}·K^{-1}

Low temperature phase— intermediate phase.

c,II/c,I	367 K,	ΔH = 49690 J·mol^{-1}
		ΔS = 7.5 J·mol^{-1}·K^{-1}

Intermediate phase— high temperaturephase.

c,I/liq	438 K,	ΔH = 7500 J·mol^{-1}
		ΔS = 17.1 J·mol^{-1}·K^{-1}

High temperature phase— isotropic liquid phase.

Molecular Weight 603.7662

Wiswesser Line Notation 14ZH 2 .ZN G4

Evaluation A

$C_{28}H_{32}Si_4O_4$ (c) 81MEK/KAR

Tetra(methylphenyl)tetrasiloxane

Heat Capacity 298.15 K, C_p = 615.0 J·mol^{-1}·K^{-1}

Temperature range 13 to 390 K.

Data given graphically.

Entropy 298.15 K, S = 662.7 J·mol^{-1}·K^{-1}

Phase Changes

c/liq	373.0 K,	ΔH = 42731 J·mol^{-1}
		ΔS = 121.8 J·mol^{-1}·K^{-1}

Molecular Weight 544.9004

Wiswesser Line Notation T8-SI-O-SI-O-SI-O-SI-O-TJ A1 AR C1 CR E1 ER G1 GR

Evaluation A

$C_{28}H_{38}N_2O_3$ (c) 83FAN/POE

4-Propionyl-4′-n-tridecanoyloxyazobenzene

Phase Changes

c/liq	374.65 K,	ΔH = 44769 J·mol^{-1}
		ΔS = 119.5 J·mol^{-1}·K^{-1}

Solid-smectic A.

Molecular Weight 450.6198

Wiswesser Line Notation 12VOR DNUNR DV2

Evaluation A

Smectic A-isotropic liquid phase change data also given:

416.65 K, ΔH = 8075 J·mol^{-1}; ΔS = 19.4 J·mol^{-1}·K^{-1}.

$C_{28}H_{40}O_4$ (liq) 81ARU/DAU

4-(2-Methylbutoxy)phenyl ester of 4-n-decycloxybenzoic acid (D)

Molecular Weight 440.6216

Wiswesser Line Notation 10OR DVOR DO1Y2&1

Evaluation C

Smectic C-smectic A, 323.7 K;

smectic A-isotropic liquid,

338.15 K, ΔS = 17.21 J·mol^{-1}·K^{-1},

phase change data given.

$C_{28}H_{58}$ (c) 55SCH/BUS

n-Octacosane

Phase Changes

c,II/c,I	331.15 K,	ΔH = 35438 J·mol^{-1}
		ΔS = 107.0 J·mol^{-1}·K^{-1}
c,I/liq	334.35 K,	ΔH = 64643 J·mol^{-1}
		ΔS = 193.3 J·mol^{-1}·K^{-1}

Molecular Weight 394.7662

Wiswesser Line Notation 28H

Evaluation B

$C_{28}H_{58}$ (c) 73COM

n-Octacosane

Phase Changes

c,II/c,I	331.25 K,	ΔH = 35438 J·mol^{-1}
		ΔS = 107.0 J·mol^{-1}·K^{-1}
c,I/liq	334.45 K,	ΔH = 64642 J·mol^{-1}
		ΔS = 193.3 J·mol^{-1}·K^{-1}

Molecular Weight 394.7662

Wiswesser Line Notation 28H

Evaluation B

$C_{29}H_{40}N_2O_3$ (c) 83FAN/POE

4-Propionyl-4′-n-tetradecanoyloxyazobenzene

Phase Changes

c/liq	375.65 K,	ΔH = 45898 J·mol^{-1}
		ΔS = 122.2 J·mol^{-1}·K^{-1}

Solid-smectic A.

Molecular Weight 464.6466

Wiswesser Line Notation 13VOR DNUNR DV2

Evaluation A

Smectic A-isotropic liquid phase change data also given:

413.65 K, ΔH = 8117 J·mol^{-1}.

$C_{29}H_{60}$ (c) 55SCH/BUS
n-Nonacosane
Phase Changes
c,II/c,I 331.35 K, ΔH = 29706 J·mol^{-1}
ΔS = 89.7 J·mol^{-1}·K^{-1}
c,I/liq 336.55 K, ΔH = 66107 J·mol^{-1}
ΔS = 196.4 J·mol^{-1}·K^{-1}
Molecular Weight 408.7930
Wiswesser Line Notation 29H
Evaluation B

$(C_{30}H_{16}N_4O_4)_n$ (c) 79KAR/SAP
Poly-(*p,p'*-diphenylenephthalido)-1,3,4-oxadiazole
Heat Capacity 298.15 K, C_p = 515.9 J·mol^{-1}·K^{-1}
Temperature range 60 to 500 K.
Entropy 298.15 K, S = 499.6 J·mol^{-1}·K^{-1}
Molecular Weight 496.4810
Wiswesser Line Notation T56 BHOVT&J BR D-CT5NN DOJ E* BR D- CT5NN DOJ ER D*/
Evaluation A

$(C_{30}H_{20}N_4O_6)_n$ (c) 79KAR/SAP
Poly-(*p,p'*-diphenylenephthalido)hydrazide
Heat Capacity 298.15 K, C_p = 583.7 J·mol^{-1}·K^{-1}
Temperature range 60 to 500 K.
Entropy 298.15 K, S = 545.6 J·mol^{-1}·K^{-1}
Molecular Weight 532.5114
Wiswesser Line Notation /T56 BHOVT&J BR DVMMVR D* BR DVMMV*/
Evaluation A

$C_{30}H_{22}$ (c) 79SMI
p-Quinquephenyl
Phase Changes
c/liq 659.6 K, ΔH = 42300 J·mol^{-1}
ΔS = 64.1 J·mol^{-1}·K^{-1}
Solid-nematic phase change.
liq/liq 688.1 K, ΔH = 922 J·mol^{-1}
ΔS = 1.34 J·mol^{-1}·K^{-1}
Nematic-isotropic phase change.
Molecular Weight 382.5038
Wiswesser Line Notation RR DR DR DR
Evaluation A

$C_{30}H_{34}O_4$ (c) 84OZC/ASR
4,4'-Diheptanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 305 K
c,II/c,I 318 K, ΔH = 18900 J·mol^{-1}
ΔS = 60.67 J·mol^{-1}·K^{-1}
c,II/c,II, c,II/c,I transitions combined.
c,I/liq 402 K, ΔH = 25500 J·mol^{-1}
ΔS = 63.47 J·mol^{-1}·K^{-1}
Solid-nematic.
Molecular Weight 458.5962
Wiswesser Line Notation 6VOR D1UU2UU1R DOV6
Evaluation A
Nematic-isotropic liquid phase change data also given:
411 K, ΔH = 1170 J·mol^{-1},
ΔS = 2.845 J·mol^{-1}·K^{-1}.

$C_{30}H_{42}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4'-*n*-pentadecanoyloxyazobenzene
Phase Changes
c/liq 376.65 K, ΔH = 51505 J·mol^{-1}
ΔS = 136.7 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 478.6734
Wiswesser Line Notation 14VOR DNUNR DV2
Evaluation A
Smectic A-isotropic liquid phase change data also given:
412.15 K, ΔH = 8452 J·mol^{-1};
ΔS = J·mol^{-1}·K^{-1}.

$C_{30}H_{46}$ (c) 83KRA/BEC
3,4-Dimethyl-3,4-bis(4-*tert*-butylphenyl)hexane
Heat Capacity 298 K, C_p = 631.3 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.371 cal·K^{-1}·g^{-1}.
Molecular Weight 406.6934
Wiswesser Line Notation 1XR DX2&2&X2&2&R DX
Evaluation B

$C_{30}H_{62}$ (c) 55SCH/BUS
n-Triacontane
Phase Changes
c,II/c,I 335.15 K
c,I/liq 338.55 K
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation B

$C_{30}H_{62}$ (c) 73COM
n-Triacontane
Phase Changes
c,II/c,I 335.25 K, ΔH = 37489 J·mol^{-1}
ΔS = 111.8 J·mol^{-1}·K^{-1}
c,I/liq 338.65 K, ΔH = 68827 J·mol^{-1}
ΔS = 203.2 J·mol^{-1}·K^{-1}
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation B

$C_{30}H_{62}$ (c) 81HOE
n-Triacontane
Heat Capacity 300 K, C_p = 558 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K.
C_v = 1.30 J·g^{-1}·K^{-1}.
Molecular Weight 422.8198
Wiswesser Line Notation 30H
Evaluation B

$C_{31}H_{44}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4'-*n*-hexadecanoyloxyazobenzene
Phase Changes
c/liq 378.65 K, ΔH = 53011 J·mol^{-1}
ΔS = 140.0 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 492.7002
Wiswesser Line Notation 15VOR DNUNR DV2
Evaluation A
Smectic A-isotropic liquid phase change data also given:
410.65 K, ΔH = 8619 J·mol^{-1};
ΔS = 21.0 J·mol^{-1}·K^{-1}.

$C_{31}H_{52}O_3$ (c) 88BAG/GUR
α-Tocopherol acetate
Heat Capacity 293.75 K, C_p = 898 J·mol^{-1}·K^{-1}
Temperature range 273 to 334 K.
Unsmoothed experimental datum.
Molecular Weight 472.7500
Wiswesser Line Notation T66 BOT&J C3Y1&3Y1&3Y1&1 C1 G1 HOV1 I1 J1
Evaluation B

$(C_{32}H_{20}N_4)_n$ (c) 74KAR/RAB
Poly-[2,2′-(p-phenylene-1,1-diphenyl-5,5′-dibenzimidazole]
Heat Capacity 298.15 K, C_p = 537.2 J·mol^{-1}·K^{-1}
Temperature range 50 to 500 K.
Entropy 298.15 K, S = 469.0 J·mol^{-1}·K^{-1}
Molecular Weight 460.5370
Wiswesser Line Notation /T56 BN DNJ CR D* H- HT56 BN DNJ CR D*& DR/
Evaluation A

$C_{32}H_2$2Ge (c) 75LEB/MIL3
1,1-Diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene
Heat Capacity 298.15 K, C_p = 556.5 J·mol^{-1}·K^{-1}
Temperature range 62 to 309 K.
Entropy 298.15 K, S = 625.1 J·mol^{-1}·K^{-1}
Molecular Weight 479.1367
Wiswesser Line Notation T5-GE- AHJ A1UU1 A1UU1 BR CR DR ER
Evaluation B

$(C_{32}H_2$2Ge$)_n$ (gls) 75LEB/MIL3
Poly-1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene
Heat Capacity 298.15 K, C_p = 489.5 J·mol^{-1}·K^{-1}
Temperature range 62 to 307 K.
Entropy 298.15 K, S = 524.7 J·mol^{-1}·K^{-1}
Molecular Weight 479.1367
Wiswesser Line Notation /T5-GE- BUTJ A1UU1 A1UU1 BR* CR* DR ER/
Evaluation B

$(C_{32}H_{24}N_4O_2)_n$ (c) 74KAR/RAB
Poly-[N-terphthalyl-bis-(N′-phenyl-o-diphenylamine)]
Heat Capacity 298.15 K, C_p = 612.1 J·mol^{-1}·K^{-1}
Temperature range 50 to 500 K.
Entropy 298.15 K, S = 601.2 J·mol^{-1}·K^{-1}
Molecular Weight 496.5674
Wiswesser Line Notation /*VMR BMR ER CMVR* DMR/
Evaluation A

$C_{32}H_{38}Fe_3N_4O_{13}$ (c) 85OH/KAM
μ_3-Oxo-tris(pyridine)hexakis(acetato) iron(II) diiron pyridine
Heat Capacity 300 K, C_p = 930 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Data given graphically.
Value estimated from graph.
Phase Changes
c,V/c,IV 111.4 K
c,IV/c,III 112.0 K
c,III/c,II 185.8 K
c,II/c,I 191.5 K
Molecular Weight 854.2122
Wiswesser Line Notation OV1 6 &T6NJ 3 &-FE- O &T6NJ
Evaluation C

$C_{32}H_{38}Fe_3N_4O_{13}$ (c) 86SOR/KAJ
μ_3-Oxo-tris(pyridine)hexakis(acetato) iron(II)-diiron pyridine
Heat Capacity 300 K, C_p = 928.91 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.
Phase Changes
c,V/c,IV 111.4 K
c,IV/c,III 112.0 K, ΔH = 503 J·mol^{-1}, ΔS = 4.61 J·mol^{-1}·K^{-1}
c,V/c,IV and c,IV/c,III combined.
c,III/c,II 185.8 K
c,II/c,I 191.5 K, ΔH = 4440 J·mol^{-1}, ΔS = 26.04 J·mol^{-1}·K^{-1}
c,III/c,II and c,II/c,I combined.
Molecular Weight 854.2122
Wiswesser Line Notation OV1 6 &T6NJ 3 &-FE- O &T6NJ
Evaluation A

$C_{32}H_{38}O_4$ (c) 84OZC/ASR
4,4′-Dioctanoyloxydinphenyldiacetylene
Phase Changes
c,II/c,I 359 K, ΔH = 35400 J·mol^{-1}, ΔS = 98.70 J·mol^{-1}·K^{-1}
c,I/liq 406 K, ΔH = 34000 J·mol^{-1}, ΔS = 83.76 J·mol^{-1}·K^{-1}
Solid-nematic.
Molecular Weight 486.6498
Wiswesser Line Notation 7VOR D1UU2UU1R DOV7
Evaluation A
Nematic-isotropic liquid phase change data also given:
412 K, ΔH = 21800 J·mol^{-1}, ΔS = 5.272 J·mol^{-1}·K^{-1}.

$C_{32}H_{39}ClO_2$ (c) 79LEW/ENE
Northindrone-6-(4-chlorophenyl)-hexanoate
Phase Changes
c/liq 413 K, ΔH = 28800 J·mol^{-1}, ΔS = 69.7 J·mol^{-1}·K^{-1}
Molecular Weight 491.1119
Wiswesser Line Notation L E5 B666 OV MUTJ E1 F1UU1 FOV5R DG
Evaluation A

$C_{32}H_{46}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-heptadecanoyloxyazobenzene
Phase Changes
c/liq 379.65 K, ΔH = 58743 J·mol^{-1}, ΔS = 154.7 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 506.7270
Wiswesser Line Notation 16VOR DNUNR DV2
Evaluation A
Smectic A-isotropic liquid phase change data also given:
409.65 K, ΔH = 8703 J·mol^{-1}; ΔS = 21.2 J·mol^{-1}·K^{-1}.

$C_{32}H_{50}$ (c) 83KRA/BEC
2,4,5,7-Tetramethyl-4,5-bis(4-*tert*-butylphenyl)octane
Heat Capacity 298 K, C_p = 683.9 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.376 cal·K^{-1}·g^{-1}.
Molecular Weight 434.7470
Wiswesser Line Notation 1XR DX1Y&X1Y&R DX
Evaluation B

$C_{32}H_{50}$ (c) 83KRA/BEC
4,5-Diethyl-4,5-bis-(4-*tert*-butylphenyl)octane
Heat Capacity 298 K, C_p = 618.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.340 cal·K^{-1}·g^{-1}.
Molecular Weight 434.7470
Wiswesser Line Notation 1XR DX2&3&X2&3&R DX
Evaluation B

$C_{32}H_{66}$ (c) 73COM
n-Dotriacontane
Phase Changes
c,II/c,I 338.65 K, ΔH = 41376 J·mol^{-1}
ΔS = 122.2 J·mol^{-1}·K^{-1}
c,I/liq 343.45 K, ΔH = 76567 J·mol^{-1}
ΔS = 222.9 J·mol^{-1}·K^{-1}
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation B

$C_{32}H_{66}$ (c) 81HOE
n-Dotriacontane
Heat Capacity 300 K, C_p = 806 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K.
C_v = 1.77 J·g^{-1}·K^{-1}.
Molecular Weight 450.8734
Wiswesser Line Notation 32H
Evaluation B

$C_{33}H_{34}O_2$ (c) 79LEW/ENE
Northindrone *trans*-4-hexylcyclohexylcarboxylate
Phase Changes
c/liq 398 K, ΔH = 22600 J·mol^{-1}
ΔS = 56.8 J·mol^{-1}·K^{-1}
Molecular Weight 462.6304
Wiswesser Line Notation L E5 B666 OV MUTJ E1
F1UU1 FOV- AL6TJ
Evaluation A

$C_{33}H_{34}O_2$ (c) 79LEW/ENE
Northindrone biphenyl-4-carboxylate
Phase Changes
c/liq 462 K, ΔH = 31600 J·mol^{-1}
Molecular Weight 462.6304
Wiswesser Line Notation L E5 B666 OV MUTJ E1
F1UU1 FOVR DR
Evaluation A

$C_{33}H_{40}O_2$ (c) 79LEW/ENE
Northindrone 4-cyclohexylbenzoate
Phase Changes
c/liq 482 K, ΔH = 36800 J·mol^{-1}
ΔS = 65.6 J·mol^{-1}·K^{-1}
Molecular Weight 468.6778
Wiswesser Line Notation L E5 B666 OV MUTJ E1
F1UU1 FOVR D- AL6TJ
Evaluation A

$C_{33}H_{48}N_2O_3$ (c) 83FAN/POE
4-Propionyl-4′-*n*-octadecanoyloxyazobenzene
Phase Changes
c/liq 380.65 K, ΔH = 59622 J·mol^{-1}
ΔS = 156.6 J·mol^{-1}·K^{-1}
Solid-smectic A.
Molecular Weight 520.7538
Wiswesser Line Notation 17VOR DNUNR DV2
Evaluation A
Smectic A-isotropic liquid phase change data also given:
408.65 K, ΔH = 8954 J·mol^{-1};
ΔS = 21.9 J·mol^{-1}·K^{-1}.

$C_{33}H_{48}O_2$ (c) 79LEW/ENE
Northindrone *trans*-3-(4-butylcyclohexyl)propionate
Phase Changes
c/liq 374 K, ΔH = 22500 J·mol^{-1}
ΔS = 60.2 J·mol^{-1}·K^{-1}
Molecular Weight 476.7410
Wiswesser Line Notation L E5 B666 OV MUTJ E1
F1UU1 FOV2- AL6TJ D4
Evaluation A

$(C_{34}H_{18}N_6O)_n$ (c) 84KAR/SHV
Polybenzimidazoloquinazole
Heat Capacity 298.15 K, C_p = 523.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 600 K.
Entropy 298.15 K, S = 453.2 J·mol^{-1}·K^{-1}
Molecular Weight 526.5560
Wiswesser Line Notation /T D6 C656 BN LNJ K* OO-
OT D6 C656 BN LNJ KR D*/
Evaluation B

$(C_{34}H_{20}N_4O)_n$ (c) 77KAR/RAB
Poly[2,2′-(1,4-phenylene)-7,7′-oxy-bis(3-phenylquinoxaline)]
Heat Capacity 300 K, C_p = 600 J·mol^{-1}·K^{-1}
Temperature range 100 to 700 K.
Data given graphically.
Value estimated from graph.
Entropy 300 K, S = 449.8 J·mol^{-1}·K^{-1}
Molecular Weight 576.6558
Wiswesser Line Notation /T66 BN ENJ CR D* HO-
HT66 BN ENJ CR DR D*/
Evaluation C(C_p,S); A(Phase changes)
T(glass) = 556.0 K.

$(C_{34}H_{22}N_6O_3)_n$ (c) 84KAR/SHV
Bis-(o-aminophenyl)-2,2′-dibenzimidazole oxide,
intermediate polymer
Heat Capacity 298.15 K, C_p = 699.2 J·mol^{-1}·K^{-1}
Temperature range 60 to 600 K.
Entropy 298.15 K, S = 594.8 J·mol^{-1}·K^{-1}
Molecular Weight 562.5864
Wiswesser Line Notation /*VR DVMR B- CT56 BM DNJ
HO- HT56 BM DNJ CR BM*/
Evaluation B

$C_{34}H_{42}O_4$ (c) 84OZC/ASR
4,4′-Dinonanoyloxydiphenyldiacetylene
Phase Changes

c,II/c,I	326 K,	ΔH = 19500 J·mol^{-1}
		ΔS = 59.79 J·mol^{-1}·K^{-1}
c,I/liq	400 K,	ΔH = 33500 J·mol^{-1}
		ΔS = 83.76 J·mol^{-1}·K^{-1}

Solid-nematic.
Molecular Weight 514.7034
Wiswesser Line Notation 8VOR D1UU2UU1R DOV8
Evaluation A
Nematic-isotropic liquid phase change data also given:
401 K, ΔH = 14600 J·mol^{-1},
ΔS = 3.640 J·mol^{-1}·K^{-1}.

$C_{34}H_{54}$ (c) 83KRA/BEC
4,5-Dipropyl-4,5-bis(4-*tert*-butylphenyl)octane
Heat Capacity 298 K, C_p = 724.2 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.374 cal·K^{-1}·g^{-1}.
Molecular Weight 462.8006
Wiswesser Line Notation 1XR DX3&3&X3&3&R DX
Evaluation B

$C_{34}H_{70}$ (c) 73COM
n-Tetratriacontane
Phase Changes

c,III/c,II	342.25 K	
c,II/c,I	342.65 K,	ΔH = 48032 J·mol^{-1}
		ΔS = 140.2 J·mol^{-1}·K^{-1}
c,I/liq	345.95 K,	ΔH = 79956 J·mol^{-1}
		ΔS = 231.1 J·mol^{-1}·K^{-1}

Molecular Weight 478.9270
Wiswesser Line Notation 34H
Evaluation B

$C_{36}H_{18}$ (c) 79FAR/SHA
Decacyclene; Diacenaphtho[1,2-j:1′,2′-l]-fluoranthene
Phase Changes

c,II/c,I	533 K	
c/liq	562.0 K,	ΔH = 45200 J·mol^{-1}
		ΔS = 80.4 J·mol^{-1}·K^{-1}

Molecular Weight 450.5382
Wiswesser Line Notation L E6 E-6 D5 P6 P-6 O5
C6566 3AC-P- K&J
Evaluation B

$C_{36}H_{46}Fe_3N_4O_{13}$ (c) 87SOR/SHI
Mixed valence iron oxo-centered complex with
acetate and 3-methyl pyridine
Heat Capacity 299.635 K, C_p = 1094.7 J·mol^{-1}·K^{-1}
Temperature range 12 to 350 K.
Unsmoothed experimental datum.
Phase Changes

c,V/c,IV	181 K
c,IV/c,III	263.5 K
c,III/c,II	271.5 K
c,II/c,I	282.2 K

Molecular Weight 910.3194
Wiswesser Line Notation -FE-3 O & T6NJ C1 3 & OV1 6 &
T6NJ C1
Evaluation A
Cumulative enthalpy and entropy changes
due to the four phase transitions were:
ΔH = 3410 J·mol^{-1},
ΔS = 13.71 J·mol^{-1}·K^{-1}.

$C_{36}H_{46}O_4$ (c) 84OZC/ASR
4,4′-Didecanoyloxydiphenyldiacetylene
Phase Changes

c,II/c,I	308 K,	ΔH = 44900 J·mol^{-1}
		ΔS = 122.1 J·mol^{-1}·K^{-1}
c,I/liq	403 K,	ΔH = 42200 J·mol^{-1}
		ΔS = 104.6 J·mol^{-1}·K^{-1}

Solid-isotropic.
Molecular Weight 542.7570
Wiswesser Line Notation 9VOR D1UU2UU1R DOV9
Evaluation A

$C_{36}H_{74}$ (c) 55SCH/BUS
n-Hexatriacontane
Phase Changes

c,III/c,II	345.25 K,	ΔH = 9916 J·mol^{-1}
		ΔS = 28.7 J·mol^{-1}·K^{-1}
c,II/c,I	346.95 K,	ΔH = 30543 J·mol^{-1}
		ΔS = 88.0 J·mol^{-1}·K^{-1}
c,I/liq	349.05 K,	ΔH = 88826 J·mol^{-1}
		ΔS = 254.5 J·mol^{-1}·K^{-1}

Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation B

$C_{36}H_{74}$ (c) 73COM
n-Hexatriacontane
Phase Changes

c,III/c,II	345.35 K,	ΔH = 9916 J·mol^{-1}
		ΔS = 28.7 J·mol^{-1}·K^{-1}
c,II/c,I	347.05 K,	ΔH = 30543 J·mol^{-1}
		ΔS = 88.0 J·mol^{-1}·K^{-1}
c,I/liq	349.15 K,	ΔH = 130666 J·mol^{-1}
		ΔS = 374.2 J·mol^{-1}·K^{-1}

Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation B

$C_{36}H_{74}$ (c) 81HOE
n-Hexatriacontane
Heat Capacity 300 K, C_p = 840 J·mol^{-1}·K^{-1}
Temperature range 300 to 500 K.
C_v = 1.64 J·g^{-1}·K^{-1}.
Molecular Weight 506.9806
Wiswesser Line Notation 36H
Evaluation B

$C_{36}H_{80}CdCl_4N_2$ (c) 84WHI
Bis(Octadecylammonium) cadmium tetrachloride
Heat Capacity 300 K, C_p = 1010 J·mol^{-1}·K^{-1}
Temperature range 10 to 370 K.
Data given graphically.
Value estimated from graph.
Phase Changes

c,V/c,IV	349.6 K,	ΔH = 49500 J·mol^{-1}
		ΔS = 132 J·mol^{-1}·K^{-1}
c,IV/c,III	356.0 K,	ΔH = 2300 J·mol^{-1}
		ΔS = 6.5 J·mol^{-1}·K^{-1}
c,III/c,II	359.5 K,	ΔH = 3500 J·mol^{-1}
		ΔS = 9.6 J·mol^{-1}·K^{-1}
c,II/c,I	365.6 K,	ΔH = 34300 J·mol^{-1}
		ΔS = 95 J·mol^{-1}·K^{-1}

Molecular Weight 795.2634
Wiswesser Line Notation 18ZH 2 .CD G4
Evaluation C(C_p); A(Phase changes)

$C_{38}H_{28}B_2F_8FeN_8$ (c) 87KUL/IYE
Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) ditetrafluoroborate
Phase Changes
c,II/c,I 280.3 K, ΔH = 15600 J·mol^{-1}; ΔS = 55.5 J·mol^{-1}·K^{-1}
Spin-state transition.
Molecular Weight 826.1470
Wiswesser Line Notation T B666 CN NNØJ D1UNMR Ø-FE-- ØT B666 CN NNØJ D1UNMR &B-F4 2
Evaluation A

$C_{38}H_{28}Cl_2FeN_8O_8$ (c) 87KUL/IYE
Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) diperchlorate
Phase Changes
c,II/c,I 244.8 K, ΔH = 15800 J·mol^{-1}; ΔS = 64.6 J·mol^{-1}·K^{-1}
Spin-state transition.
Molecular Weight 851.4410
Wiswesser Line Notation T B666 CN NNØJ D1UNMR Ø-FE-- ØT B666 CN NNØJ D1UNMR &G-O4 2
Evaluation A

$C_{38}H_{36}O_4Si_4$ (c) 82KUL
1,1,3,3,5,5-Hexaphenyl-7,7-dimethylcyclotetrasiloxane
Heat Capacity 298.15 K, C_p = 815.5 J·mol^{-1}·K^{-1}
Temperature range 12 to 340 K.
Entropy 298.15 K, S = 865.7 J·mol^{-1}·K^{-1}
Molecular Weight 669.0420
Wiswesser Line Notation T8-SI-O-SI-O-SI-OJ AR AR C1 C1 ER ER GR GR
Evaluation A

$C_{38}H_{50}O_4$ (c) 84OZC/ASR
4,4'-Diundecanoyloxydiphenyldiacetylene
Phase Changes
c,III/c,II 339 K, ΔH = 18100 J·mol^{-1}; ΔS = 53.54 J·mol^{-1}·K^{-1}
c,II/c,I 359 K, ΔH = 7590 J·mol^{-1}; ΔS = 21.14 J·mol^{-1}·K^{-1}
c,I/liq 399 K, ΔH = 36200 J·mol^{-1}; ΔS = 90.85 J·mol^{-1}·K^{-1}
Solid-isotropic.
Molecular Weight 570.8106
Wiswesser Line Notation 10OVR D1UU2UU1R DOV10
Evaluation A

$C_{38}H_{62}$ (c) 83KRA/BEC
5,6-Dibutyl-5,6-bis(4-*tert*-butylphenyl)decane
Heat Capacity 298 K, C_p = 805.5 J·mol^{-1}·K^{-1}
One temperature.
C_p given as 0.371 cal·K^{-1}·g^{-1}.
Molecular Weight 518.9078
Wiswesser Line Notation 1XR DX4&4&X4&4&R DX
Evaluation B

$(C_{38}H_{70}O_8)_n$ (liq) 75PHI/WAL
Poly(hexamethylene sebacate)
Heat Capacity 328.15 K, C_p = 1290 J·mol^{-1}·K^{-1}
Temperature range 328.15 to 408.15 K.
Phase Changes
c/liq 306 K
Molecular Weight 654.9662
Wiswesser Line Notation 60V8VO6VO8VO6
Evaluation B

$C_{39}H_{30}N_6$ (c) 84LEB/BYK
Hexaphenylisomelamine
Heat Capacity 298.15 K, C_p = 672.4 J·mol^{-1}·K^{-1}
Temperature range 8 to 330 K.
Entropy 298.15 K, S = 706.5 J·mol^{-1}·K^{-1}
Molecular Weight 582.7062
Wiswesser Line Notation T6NYNYNYJ AR BUNR CR DUNR ER FUNR
Evaluation A

$C_{39}H_{30}N_6$ (c) 84LEB/BYK
Hexaphenylmelamine
Heat Capacity 298.15 K, C_p = 665.8 J·mol^{-1}·K^{-1}
Temperature range 10 to 330 K.
Entropy 298.15 K, S = 673.7 J·mol^{-1}·K^{-1}
Molecular Weight 582.7062
Wiswesser Line Notation T6N CN ENJ BNR&R DNR&R FNR&R
Evaluation A

$C_{40}H_{54}O_4$ (c) 84OZC/ASR
4,4'-Didodecanoyloxydiphenyldiacetylene
Phase Changes
c,II/c,I 374 K, ΔH = 50200 J·mol^{-1}; ΔS = 134.1 J·mol^{-1}·K^{-1}
c,I/liq 401 K, ΔH = 44000 J·mol^{-1}; ΔS = 109.7 J·mol^{-1}·K^{-1}
Solid-isotropic.
Molecular Weight 598.8642
Wiswesser Line Notation 11OVR D1UU2UU1R DOV11
Evaluation A

$C_{41}H_{72}O_2$ (c) 86KIS/IWA
Cholesteryl myristate
Phase Changes
c,I/liq 344.6 K, ΔH = 47100 J·mol^{-1}
Solid-smectic transition.
liq/liq 353.0 K, ΔH = 1600 J·mol^{-1}
Smectic-cholesteric.
liq/liq 358.3 K, ΔH = 1100 J·mol^{-1}
Cholesteric-isotropic.
Molecular Weight 597.0186
Wiswesser Line Notation L E5 B666 LUTJ A1 E1FY1&3Y1&1 OV13
Evaluation A

$C_{42}H_{66}O_{12}$ (c) 79SOR/TSU
Benzene-hexa-*n*-hexanoate
Heat Capacity 300 K, C_p = 1300 J·mol^{-1}·K^{-1}
Temperature range 13 to 393 K.
Data given graphically.
C_p value is a graphical estimate.
Phase Changes
c,IV/c,III 251.58 K, ΔH = 25660 J·mol^{-1}; ΔS = 102.67 J·mol^{-1}·K^{-1}
c,III/c,II 291.46 K, ΔH = 12270 J·mol^{-1}; ΔS = 46.11 J·mol^{-1}·K^{-1}
c,II/c,I 348.27 K, ΔH = 16260 J·mol^{-1}; ΔS = 46.68 J·mol^{-1}·K^{-1}
c,I/liq 368.74 K, ΔH = 33500 J·mol^{-1}; ΔS = 90.86 J·mol^{-1}·K^{-1}
Molecular Weight 762.9762
Wiswesser Line Notation 5OVR BVO5 CVO5 DVO5 EVO5 FVO5
Evaluation B(C_p); A(Phase changes)

$C_{42}H_{70}O_{35}\cdot 11H_2O$ (c) 87HAN/MAT

β-Cyclodextrin undecahydrate; Cycloheptaamylose undecahydrate

Heat Capacity 299.53 K, C_p = 2093 J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Unsmoothed experimental datum.

Phase Changes

c,II/c,I 226 K, ΔS = 45.0 J·mol^{-1}·K^{-1}

Molecular Weight 1333.1612

Wiswesser Line Notation /T5OTJ B* CQ DQ EO* F1Q/ 7

Evaluation A
T(glass) = 150 K.

$C_{42}H_{72}O_{12}$ (c) 84KOH/PRA

Hexa-O-hexanoyl-scyllo-inositol

Phase Changes

c/liq 341.6 K, ΔH = 21150 J·mol^{-1}
ΔS = 61.9 J·mol^{-1}·K^{-1}
Solid-discotic.

liq/liq 472.6 K, ΔH = 8840 J·mol^{-1}
ΔS = 18.7 J·mol^{-1}·K^{-1}
Discotic-isotropic.

Molecular Weight 769.0236

Wiswesser Line Notation L6TJ AOV5 BOV5 COV5 DOV5 EOV5 FOV5

Evaluation A

$C_{43}H_{26}N_8P$ (c) 70KOS/IID

Methyltriphenylphosphonium-bis(7,7,8,8-tetracyanoquinodimethanide)

Heat Capacity 300 K, C_p = 858 J·mol^{-1}·K^{-1}
Temperature range 5 to 350 K.
Data given graphically only.
Value estimated from graph.

Molecular Weight 685.7058

Wiswesser Line Notation L6Y DYJ AYCN&CN DYCN&CN 2 &1PR&R&R

Evaluation C

$C_{43}H_{76}O_2$ (c) 86KIS/IWA

Cholesteryl palmitate

Phase Changes

c,I/liq 350.4 K, ΔH = 56200 J·mol^{-1}
ΔS = 160.4 J·mol^{-1}·K^{-1}
Solid-smectic transition.

liq/liq 349.9 K, ΔH = 1700 J·mol^{-1}
ΔS = 4.86 J·mol^{-1}·K^{-1}
Smectic-cholesteric.

liq/liq 355.0 K, ΔH = 1300 J·mol^{-1}
ΔS = 3.66 J·mol^{-1}·K^{-1}
Cholesteric-isotropic.

Molecular Weight 625.0722

Wiswesser Line Notation L E5 B666 LUTJ A1 E1FY1&3Y1&1 OV15

Evaluation A

$C_{45}H_{78}O_2$ (c) 86KIS/IWA

Cholesteryl oleate

Phase Changes

c,I/liq 321.1 K, ΔH = 2900 J·mol^{-1}
ΔS = 9.03 J·mol^{-1}·K^{-1}
Solid$_1$-isotropic.
Solid$_2$-isotropic also given:
317.4 K, ΔH = 2700 J·mol^{-1};
ΔS = 8.51 J·mol^{-1}·K^{-1}.

liq/liq 315.9 K, ΔH = 1300 J·mol^{-1}
ΔS = 4.12 J·mol^{-1}·K^{-1}
Smectic-cholesteric.

liq/liq 321.0 K, ΔH = 840 J·mol^{-1}
ΔS = 2.62 J·mol^{-1}·K^{-1}
Cholesteric-isotropic.

Molecular Weight 651.1100

Wiswesser Line Notation L E5 B666 LUTJ A1 E1FY1&3Y1&1 OV8U9

Evaluation A

$C_{45}H_{80}O_2$ (c) 86KIS/IWA

Cholesteryl stearate

Phase Changes

c,I/liq 355.4 K, ΔH = 67500 J·mol^{-1}
ΔS = 189.9 J·mol^{-1}·K^{-1}
Solid-isotropic.

liq/liq 349.0 K, ΔH = 1800 J·mol^{-1}
ΔS = 5.16 J·mol^{-1}·K^{-1}
Smectic-cholesteric.

liq/liq 353.0 K, ΔH = 1700 J·mol^{-1}
ΔS = 4.82 J·mol^{-1}·K^{-1}
Cholesteric-isotropic.

Molecular Weight 653.1258

Wiswesser Line Notation L E5 B666 LUTJ A1 E1FY1&3Y1&1 OV17

Evaluation A

$C_{48}H_{40}O_4Si_4$ (c) 82KUL

Octaphenylcyclotetrasiloxane

Heat Capacity 298.15 K, C_p = 932.5 J·mol^{-1}·K^{-1}
Temperature range 12 to 300 K.

Entropy 298.15 K, S = 1044 J·mol^{-1}·K^{-1}

Molecular Weight 793.1836

Wiswesser Line Notation T8SIOSIOSIOSIOJ AR AR CR CR ER ER GR GR

Evaluation A

$C_{48}H_{78}O_{12}$ (c) 79SOR/TSU

Benzene-hexa-*n*-heptanoate

Heat Capacity 300 K, C_p = 1500 J·mol^{-1}·K^{-1}
Temperature range 13 to 393 K.
Data given graphically.
C_p value is a graphical estimate.

Phase Changes

c,IV/c,III 129 K, ΔH = 1120 J·mol^{-1}
ΔS = 8.46 J·mol^{-1}·K^{-1}

c,III/c,II 222.80 K

c,II/c,I 230.81 K, ΔH = 11500 J·mol^{-1}
ΔS = 50.44 J·mol^{-1}·K^{-1}
Combination of transition c,III/c,II and c,II/c,I.

c,I/liq 353.79 K, ΔH = 32210 J·mol^{-1}
ΔS = 91.08 J·mol^{-1}·K^{-1}
Solid-mesophase.

Molecular Weight 847.1370

Wiswesser Line Notation 6OVR BVO6 CVO6 DVO6 EVO6 FVO6

Evaluation A(Phase changes), B(C_p)
Mesophase-liquid phase transition data also given:
359.28 K, ΔH = 21540 J·mol^{-1},
ΔS = 59.93 J·mol^{-1}·K^{-1}.

$C_{54}H_{90}O_{12}$ (c) 82SOR/YOS
Benzene hexa-*n*-octanoate
Heat Capacity 298.15 K, C_p = 2131.3 J·mol^{-1}·K^{-1}
Temperature range 13 to 393 K.
Entropy 298.15 K, S = 1514.3 J·mol^{-1}·K^{-1}
Phase Changes
c,II/c,I 301.89 K, ΔH = 48960 J·mol^{-1}
ΔS = 164.01 J·mol^{-1}·K^{-1}
c,I/liq 355.10 K, ΔH = 46070 J·mol^{-1}
ΔS = 129.81 J·mol^{-1}·K^{-1}
Solid-columnar mesophase.
Molecular Weight 931.2978
Wiswesser Line Notation 7VOR BOV7 COV7 DOV7 EOV7 FOV7
Evaluation A
Columnar mesophase-isotropic liquid phase change data also given:
357.09 K, ΔH = 19220 J·mol^{-1},
ΔS = 53.77 J·mol^{-1}·K^{-1}.

$C_{54}H_{96}O_{12}$ (c) 84KOH/PRA
Hexa-O-octanoyl-scyllo-inositol
Phase Changes
c/liq 348.6 K, ΔH = 43330 J·mol^{-1}
ΔS = 124.3 J·mol^{-1}·K^{-1}
Solid-discotic.
liq/liq 471.6 K, ΔH = 9470 J·mol^{-1}
ΔS = 20.08 J·mol^{-1}·K^{-1}
Discotic-isotropic.
Molecular Weight 937.3452
Wiswesser Line Notation H6TJ AOV7 BOV7 COV7 DOV7 EOV7 FOV7
Evaluation A

$C_{54}H_{98}O_{12}$ (liq) 75PHI/WAL
Poly(hexamethylene sebacate)
Heat Capacity 333.15 K, C_p = 1850 J·mol^{-1}·K^{-1}
Temperature range 333.15 to 433.15 K.
Phase Changes
c/liq 322 K
Molecular Weight 939.3610
Wiswesser Line Notation 6OV8VO6VO8VO6VO8VO6
Evaluation B

$C_{54}H_{104}O_6$ (c) 84SIM/HOC
Trimargarin; Glyceryl trimargarate
Heat Capacity 300 K
Temperature range 190 to 350 K.
Heat capacity given for the following solid state phases:
(J·mol^{-1}·K^{-1}); β (mp, 338 K) = 1393;
β_1'(mp, 335 K) 1518; β_2'(mp, 333 K) = 1621;
α (mp, 323 K) = 1759.
Molecular Weight 849.4120
Wiswesser Line Notation 16VO1YOV16&1OV16
Evaluation B

$C_{57}H_{110}O_6$ (c) 84SIM/HOC
Tristearin; Glyceryl tristearate
Heat Capacity 300 K
Temperature range 190 to 350 K.
Heat capacity given for the following solid state phases:
(J·mol^{-1}·K^{-1}); β (mp, 345 K) = 1436;
β_1'(mp, 337 K) = 1544; β_2'(mp, 334 K) = 1615;
α (mp, 328 K) = 1846.
Molecular Weight 891.4924
Wiswesser Line Notation 17VO1YOV17&1OV17
Evaluation B

$C_{66}H_{96}O_{12}$ (c) 86HEC/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
(Solid I)
Heat Capacity 298.651 K, C_p = 2016.6 J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K.
Unsmoothed experimental datum.
Phase Changes
c,I/liq 362.6 K, ΔH = 24210 J·mol^{-1}
ΔS = 66.76 J·mol^{-1}·K^{-1}
Crystal/discotic.
liq/liq 402.16 K, ΔH = 3626 J·mol^{-1}
ΔS = 9.02 J·mol^{-1}·K^{-1}
Discotic/Isotropic liquid.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J COV8 DOV8 IOV8 JOV8 OOV8 POV8
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86HEC/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
(Solid II)
Heat Capacity 299.036 K, C_p = 2082.0 J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K.
Unsmoothed experimental datum.
Phase Changes
c,II/liq 359.7 K, ΔH = 25440 J·mol^{-1}
ΔS = 71.12 J·mol^{-1}·K^{-1}
Crystal/discotic.
liq/liq 402.16 K, ΔH = 3626 J·mol^{-1}
ΔS = 9.02 J·mol^{-1}·K^{-1}
Discotic/isotropic liquid.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J COV8 DOV8 IOV8 JOV8 OOV8 POV8
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86HEC/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
(Solid III)
Heat Capacity 298.428 K, C_p = 1956.1 J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K.
Unsmoothed experimental datum.
Phase Changes
c,III/c,I 290 K, ΔH = 15320 J·mol^{-1}
ΔS = 52.8 J·mol^{-1}·K^{-1}
Expected phase transition, but not observed.
c,III/liq 348 K, ΔH = 34770 J·mol^{-1}
ΔS = 99.91 J·mol^{-1}·K^{-1}
Crystal/discotic.
liq/liq 402.16 K, ΔH = 3626 J·mol^{-1}
ΔS = 9.02 J·mol^{-1}·K^{-1}
Discotic/isotropic liquid.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J COV8 DOV8 IOV8 JOV8 OOV8 POV8
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86VAN/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Heat Capacity 298.651 K, $C_p = 2016.6$ J·mol^{-1}·K^{-1}
Temperature range 12 to 365 K.
Unsmoothed experimental datum for "Solid-I".
Phase Changes
c/liq 362.6 K, $\Delta H = 24210$ J·mol^{-1}
$\Delta S = 66.76$ J·mol^{-1}·K^{-1}
Solid I—discotic.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J EOV7 FOV7 KOV7 LOV7 QOV7 ROV7
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86VAN/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Heat Capacity 299.036 K, $C_p = 2082.0$ J·mol^{-1}·K^{-1}
Temperature range 12 to 425 K.
Unsmoothed experimental datum for "solid-II".
Phase Changes
liq/liq 402.16 K, $\Delta H = 3626$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Discotic— isotropic.
c/liq 359.7 K, $\Delta H = 25440$ J·mol^{-1}
$\Delta S = 71.12$ J·mol^{-1}·K^{-1}
Solid II—discotic.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J EOV7 FOV7 KOV7 LOV7 QOV7 ROV7
Evaluation A

$C_{66}H_{96}O_{12}$ (c) 86VAN/KAJ
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
Heat Capacity 298.428 K, $C_p = 1956.1$ J·mol^{-1}·K^{-1}
Temperature range 12 to 348 K.
Unsmoothed experimental datum for "Solid-III".
Phase Changes
c/liq 348 K, $\Delta H = 34770$ J·mol^{-1}
$\Delta S = 9.02$ J·mol^{-1}·K^{-1}
Solid III—discotic.
Molecular Weight 1081.4772
Wiswesser Line Notation L B6 H666J EOV7 FOV7 KOV7 LOV7 QOV7 ROV7
Evaluation A

$C_{66}H_{120}O_{12}$ (c) 84KOH/PRA
Hexa-O-decanoyl-scyllo-inositol
Phase Changes
c/liq 357.1 K, $\Delta H = 53070$ J·mol^{-1}
$\Delta S = 148.6$ J·mol^{-1}·K^{-1}
Solid-discotic.
liq/liq 461.8 K, $\Delta H = 10280$ J·mol^{-1}
$\Delta S = 22.26$ J·mol^{-1}·K^{-1}
Discotic-isotropic.
Molecular Weight 1105.6668
Wiswesser Line Notation L6TJ AOV9 BOV9 COV9 DOV9 EOV9 FOV9
Evaluation A

$C_{203}H_{288}O_{14}$ (c) 87AWA/SUG
Galvinoxyl hydrogalvinoxyl (6:1) radical
Heat Capacity 299.62 K, $C_p = 634.81$ J·mol^{-1}·K^{-1}
Temperature range 12 to 303 K.
Unsmoothed experimental datum.
Molecular Weight 2952.4998
Wiswesser Line Notation
Evaluation A

$C_{290}H_{411}O_{20}$ (c) 87AWA/SUG
Galvinoxyl hydrogalvinoxyl (9:1) radical
Heat Capacity 298.45 K, $C_p = 631.92$ J·mol^{-1}·K^{-1}
Temperature range 13 to 300 K.
Unsmoothed experimental datum.
Phase Changes
c,II/c,I 71 K, $\Delta H = 718$ J·mol^{-1}
$\Delta S = 10.11$ J·mol^{-1}·K^{-1}
Diamagnetic low temperature- paramagnetic high temperature phase transition in 9:1 crystal.
Molecular Weight 4217.4249
Wiswesser Line Notation
Evaluation A

8. Compound Name — Formula Index

A

B

Bis(nitrato)(1,4,8,11-tetraazacyclotetradecane) copper (II)	$C_{10}H_{24}CuN_6O_6$
Bis-pentylammonium tetrachloro zincate	$C_{10}H_{28}Cl_4N_2Zn$
Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) ditetrafluoroborate	$C_{38}H_{28}B_2F_8FeN_8$
Bis(1,10-phenanthroline-2-carbaldehyde phenylhydrazone) iron(II) diperchlorate	$C_{38}H_{28}Cl_2FeN_8O_8$
2,2-Bis(phenyl-4-glycidoxy)propane	$C_{21}H_{24}O_4$
1,4-Bis(phenylglyoxaloyl)benzene	$C_{22}H_{14}O_4$
Bis(tetradecylammonium)zinc tetrachloride	$C_{28}H_{32}Cl_4N_2Zn$
Bis(tetraethylammonium) decahydrodecaborate	$C_{16}H_{50}B_{10}N_2$
Bis(tetraethylammonium) dodecahydrododecaborate	$C_{16}H_{52}B_{12}N_2$
Bis(tetramethylammonium iodide) trideca-silver iodide	$C_8H_{24}Ag_{13}I_{15}N_2$
Bis(toluene)chromium iodide	$C_{14}H_{16}CrI$
o,o′-Bis-trichlorosilylbiphenyl	$C_{12}H_8Cl_4Si_2$
1,3-Bis(trimethylsilyl)propane	$C_9H_{24}Si_2$
Bis(m-xylene)chromium iodide	$C_{16}H_{20}CrI$
2,2′-Bitetralin	$C_{20}H_{22}$
Bromo bis(N,N-diethyldithiocarbamate)iron (III)	$C_{10}H_{20}BrFeN_2S_4$
Bromobenzene	C_6H_5Br
2-Bromobenzoic acid	$C_7H_5BrO_2$
3-Bromobenzoic acid	$C_7H_5BrO_2$
4-Bromobenzoic acid	$C_7H_5BrO_2$
1-Bromo-2-chloro-1,1,2-trifluoroethane	$C_2HBrClF_3$
2-Bromo-2-chloro-1,1,1-trifluoroethane	$C_2HBrClF_3$
Bromoform	$CHBr_3$
2-Bromoiodobenzene	C_6H_4BrI
3-Bromoiodobenzene	C_6H_4BrI
4-Bromoiodobenzene	C_6H_4BrI
4-Bromophenol	C_6H_5BrO
Bromotrifluoromethane	CF_3Br
Bullvalene	$C_{10}H_{10}$
Butadiene-propylene copolymer	$(C_7H_{12})_n$
1,4-Butanedinitrile	$C_4H_4N_2$
1,4-Butanedioic acid	$C_6H_{10}O_4$
1,4-Butanediol	$C_4H_{10}O_2$
1-Butanethiol	$C_4H_{10}S$
1-Butanol	$C_4H_{10}O$
2-Butanol	$C_4H_{10}O$
tert-Butanol	$C_4H_{10}O$
Butanone	C_4H_8O
2-Butenal	C_4H_6O
1-Butene	C_4H_8
cis-2-Butene	C_4H_8
trans-2-Butene	C_4H_8
2-*n*-Butoxy-1-ethanol	$C_6H_{14}O_2$
2-(2-Butoxyethoxy)ethanol	$C_8H_{18}O_3$
n-Butyl acetate	$C_6H_{12}O_2$
Butyl acrylate	$C_7H_{12}O_2$
n-Butyl alcohol	$C_4H_{10}O$
sec-Butyl alcohol	$C_4H_{10}O$
tert-Butyl alcohol	$C_4H_{10}O$
Butyl butanoate	$C_8H_{16}O_2$
n-Butyl chloride	C_4H_9Cl
n-Butyl ethanoate	$C_6H_{12}O_2$
n-Butyl mercaptan	$C_4H_{10}S$
Butyl methacrylate	$C_8H_{14}O_2$
n-Butyl methanoate	$C_5H_{10}O_2$
Butyl octadecanoate	$C_{12}H_{24}O_2$
Butyl pentanoic acid	$C_9H_{18}O_2$
Butyl urea	$C_5H_{12}N_2O$
tert-Butyl urea	$C_5H_{12}N_2O$
tert-Butylaldehyde	$C_5H_{10}O$
1,4-Butylene glycol-ethylene glycol-adipic acid oligomer	$C_{12}H_{22}O_6$
Butylglycol	$C_6H_{14}O_2$
τ-Butyrolactone	$C_4H_6O_2$

C

Caffeine	$C_8H_{10}N_4O_2$
Calcium oxalate mono-hydrate	$C_2CaO_4{\cdot}H_2O$
Cane sugar	$C_{12}H_{22}O_{11}$
Capraldehyde	$C_{10}H_{20}O$
Capric acid	$C_{10}H_{20}O_2$
Capric aldehyde	$C_{10}H_{20}O$
ϵ-Caprolactone	$C_6H_{10}O_2$
Capryl alcohol	$C_8H_{18}O$
Caprylaldehyde	$C_8H_{16}O$
4-Carbomethoxyhomocubane	$C_{11}H_{12}O_2$
Carbon	C
Carbon, diamond	C
Carbon, graphite	C
Carbon tetrabromide	CBr_4
Carbon tetrachloride	CCl_4
Carbon tetrafluoride	CF_4
Carbopropoxy methyl methacrylate	$C_9H_{14}O_2$
1,7-Carborane-12	$C_2H_{12}B_{10}$
m-Carborane	$C_2H_{12}B_{10}$
4-Carboxypentacyclo-[4.3.0.0^{2,5}.0^{3,8}.0^{4,7}]nonane	$C_{10}H_{10}O_2$
Castor oil	$C_{18}H_{34}O_3$
Catechol	$C_6H_6O_2$
Cellulose nitrate	$(C_6H_8N_2O_9)_n$
Cerium(III) oxalate	$C_6O_{12}Ce_2$
n-Cetyl alcohol	$C_{16}H_{34}O$
Cetane	$C_{16}H_{34}$
2-Chloro-1-(trichloromethyl)pyridine	$C_6H_3Cl_4N$
Chloroacetic acid	$C_2H_3ClO_2$
2-Chloroadamantane	$C_{10}H_{15}Cl$
Chlorobenzene	C_6H_5Cl
p-Chlorobiphenyl	$C_{12}H_9Cl$
Chlorobis(N,N-dimethyldithiocarbamate)iron(III)	$C_6H_{12}ClFeN_2S_4$
2-Chlorobromobenzene	C_6H_4BrCl
3-Chlorobromobenzene	C_6H_4BrCl
4-Chlorobromobenzene	C_6H_4BrCl
1-Chlorobutane	C_4H_9Cl
Chloroethyl methacrylate	$C_6H_9ClO_2$
Chloroform	$CHCl_3$
2-Chloroisonitrosoacetanilide	$C_8H_7ClN_2O_2$
1-Chloronaphthalene	$C_{10}H_7Cl$
2-Chloronaphthalene	$C_{10}H_7Cl$
1,2-Chloronitrobenzene	$C_6H_4ClNO_2$
2-Chlorophenol	C_6H_5ClO
3-Chlorophenol	C_6H_5ClO
4-Chlorophenol	C_6H_5ClO
Chlorotrifluoroethylene	C_2ClF_3
Chlorotrifluoroethene	C_2ClF_3
Chlorotrimethylsilane	C_3H_9ClSi
Cholesteryl oleate	$C_{45}H_{78}O_2$
Cholesteryl myristate	$C_{41}H_{72}O_2$
Cholesteryl palmitate	$C_{43}H_{76}O_2$
Cholesteryl stearate	$C_{45}H_{80}O_2$
Chroman	C_9H_7O
Chromium acetylacetonate	$C_{15}H_{21}CrO_6$
Chromocene	$C_{10}H_{10}Cr$
Cinnamic acid	$C_9H_8O_2$
Citral	$C_{10}H_{16}O$
Citric acid monohydrate	$C_6H_8O_7{\cdot}H_2O$
Citric acid	$C_6H_8O_7$

Cobaltocene	$C_{10}H_{10}Co$
Copper benzylacetylenide	C_9H_7Cu
Copper butylacetylenide	C_6H_9Cu
Copper (II) formate tetradeuterate	$C_2H_2CuO_4{\cdot}4D_2O$
Copper (II) formate tetrahydrate	$C_2H_2CuO_4{\cdot}4H_2O$
Copper phenylacetylenide	C_8H_5Cu
Copper phenylethynylacetylenide	$C_{10}H_5Cu$
Copper vinylacetylenide	C_4H_3Cu
o-Cresol	C_7H_8O
m-Cresol	C_7H_8O
p-Cresol	C_7H_8O
Crotonaldehyde	C_4H_6O
Cyanamid	CH_2N_2
Cyanoacetamide	$C_3H_4N_2O$
α-Cyanopropionaldehyde	C_4H_5NO
β-Cyanopropionaldehyde	C_4H_5NO
Cyanuric acid	$C_3H_3N_3O_3$
Cyclam	$C_{10}H_{24}N_4$
β-Cyclodextrin undecahydrate	$C_{42}H_{70}O_{35}{\cdot}11H_2O$
Cyclo-di-p-xylene	$C_{16}H_{16}$
Cycloheptaamylose undecahydrate	$C_{42}H_{70}O_{35}{\cdot}11H_2O$
cis-Cycloheptene	C_7H_{12}
cis-Cyclohexane-1,2-dicarboxylic-anhydride	$C_8H_{10}O_3$
Cyclohexane	C_6H_{12}
1,4-Cyclohexanedione	$C_6H_8O_2$
Cyclohexanone	$C_6H_{10}O$
(Cyclohexatriene)(cyclopentadienyl)-iron(II) hexafluorophosphate	$C_{11}H_{11}F_6FeP$
Cyclohexene	C_6H_{10}
Cyclohexene oxide	$C_6H_{10}O$
Cyclohexylbenzene	$C_{12}H_{16}$
Cyclooctadecane	$C_{18}H_{36}$
Cycloocta-1,5-diene	C_8H_{12}
Cyclooctane	C_8H_{16}
Cyclooctene	C_8H_{14}
Cyclopentadiene	C_5H_6
Cyclopentadienyl manganese tricarboxyl	$C_8H_5MnO_3$
Cymantrene	$C_8H_5MnO_3$

D

Decachlorobiphenyl	$C_{12}Cl_{10}$
Decacyclene	$C_{36}H_{18}$
Decafluorobiphenyl	$C_{12}F_{10}$
cis-Decahydronaphthalene	$C_{10}H_{18}$
trans-Decahydronaphthalene	$C_{10}H_{18}$
Decanal	$C_{10}H_{20}O$
Decane	$C_{10}H_{22}$
n-Decane	$C_{10}H_{22}$
1-Decanethiol	$C_{10}H_{22}S$
cis-Decalin	$C_{10}H_{18}$
trans-Decalin	$C_{10}H_{18}$
Decanoic acid	$C_{10}H_{20}O_2$
n-Decyl mercaptan	$C_{10}H_{22}S$
Decyl methacrylate	$C_{14}H_{26}O_2$
Decylcyanobiphenyl	$C_{23}H_{29}N$
Deuterotriglycine fluoroberyllate	$C_6D_{17}BeF_4N_3O_6$
Deuterotriglycine sulfate	$C_6D_{17}N_3O_{10}S$
Diacenaphtho[1,2-j:1′,2′-l]fluoranthene	$C_{36}H_{18}$
p-Diacetylbenzene diethyl ketal	$C_{18}H_{30}O_4$
4,4′-Diaminodiphenyl ether	$C_{12}H_{12}N_2O$
4,4′-Diaminodiphenyl oxide	$C_{12}H_{12}N_2O$
4,4′-Diaminodiphenyl sulfone	$C_{12}H_{12}N_2O_2S$
Diamond	C
1,2-Diaminoethane	$C_2H_8N_2$
2,3-Diazabicyclo[2.2.2]oct-2-ene N-oxide	$C_6H_{10}N_2O$
6,7-Diazatricyclo[3.2.2.0^{2,4}]non-6-ene N-oxide	$C_7H_{10}N_2O$
1,2,3,4-Dibenzanthracene picric acid	$C_{28}H_{17}N_3O_7$
1,2,5,6-Dibenzanthracene picric acid	$C_{28}H_{17}N_3O_7$
Dibenzothiophene	$C_{12}H_8S$
1,2-Dibromobenzene	$C_6H_4Br_2$
1,3-Dibromobenzene	$C_6H_4Br_2$
1,4-Dibromobenzene	$C_6H_4Br_2$
1,4-Dibromo-2,3-dichorohexa-fluorobutane	$C_4Br_2Cl_2F_6$
1,2-Dibromoethane	$C_2H_4Br_2$
1,6-Dibromo-2,3,5-trichloro-nonafluorohexane	$C_6Br_2Cl_3F_9$
1,2-Dibromotetrafluoroethane	$C_2Br_2F_4$
4,4′-Dibutanoyloxydi-phenyldiacetylene	$C_{24}H_{22}O_4$
Di-*n*-butyl ether	$C_8H_{18}O$
Di-*tert*-butyl ether	$C_8H_{18}O$
5,6-Dibutyl-5,6-bis(4-*tert*-butyl-phenyl)decane	$C_{38}H_{62}$
Dibutyl phthalate	$C_{16}H_{22}O_4$
Dibutyl *o*-phthalate	$C_{16}H_{22}O_4$
N,N′-Dibutylurea	$C_9H_{20}N_2O$
Dichloroacetic acid	$C_2H_2Cl_2O_2$
1,2-Dichlorobenzene	$C_6H_4Cl_2$
1,3-Dichlorobenzene	$C_6H_4Cl_2$
1,4-Dichlorobenzene	$C_6H_4Cl_2$
p-Dichlorobenzene	$C_6H_4Cl_2$
p-Dichlorobenzophenone	$C_{13}H_8Cl_2O$
1,4-Dichlorobutane	$C_4H_8Cl_2$
4,4′-Dichlorodiphenyl sulphone	$C_{12}H_8Cl_2O_2S$
1,2-Dichloroethane	$C_2H_4Cl_2$
Dichloroethanoic acid	$C_2H_2Cl_2O_2$
1,6-Dichlorohexane	$C_6H_{12}Cl_2$
Dichloromethane	CH_2Cl_2
Dichlorodimethylsilane	$C_2H_6Cl_2Si$
Dichloromethylvinylsilane	$C_3H_6Cl_2Si$
2,4-Dichloro-4′-nitrodiphenyl ether	$C_{12}H_7Cl_2NO_3$
2,3-Dichlorophenol	$C_6H_4Cl_2O$
2,4-Dichlorophenol	$C_6H_4Cl_2O$
2,5-Dichlorophenol	$C_6H_4Cl_2O$
2,6-Dichlorophenol	$C_6H_4Cl_2O$
3,4-Dichlorophenol	$C_6H_4Cl_2O$
3,5-Dichlorophenol	$C_6H_4Cl_2O$
1,2-Dicyanobenzene	$C_8H_4N_2$
1,4-Dicyanobenzene	$C_8H_4N_2$
1,1-Dicyclohexyldodecane	$C_{24}H_{46}$
endo-Dicyclopentadiene	$C_{10}H_{12}$
4,4′-Didecanoyloxydiphenyl-diacetylene	$C_{36}H_{46}O_4$
Di-*n*-decylammonium chloride	$C_{20}H_{44}ClN$
4,4′-Didodecanoyloxydiphenyl-diacetylene	$C_{40}H_{54}O_4$
Diethanolamine	$C_4H_{11}NO_2$
4,4′-Diethanoyloxydiphenyldiacetylene	$C_{20}H_{14}O_4$
Diethylaminoethyl methacrylate	$C_{10}H_{19}NO_2$
4,5-Diethyl-4,5-bis-(4-*tert*-butyl-phenyl)octane	$C_{32}H_{50}$
Diethylene glycol	$C_4H_{10}O_3$
Diethylene glycol-glycerol-adipate polymer	$C_{13}H_{22}O_8$
Diethylene glycol-trimethylolpro-pane-adipate polymer	$C_{15}H_{28}O_8$
Diethyleneimide oxide	C_4H_9NO
Diethylenetriamine	$C_3H_{13}N_3$
Di-(2-ethylhexyl)adipate	$C_{22}H_{42}O_4$
Di-(2-ethylhexyl) *o*-phthalate	$C_{24}H_{38}O_4$
Diethyl ketone	$C_5H_{10}O$
Diethyl mercury	$C_4H_{10}Hg$
3,3-Diethylpentane	C_9H_{20}
N,N-Diethylurea	$C_5H_{12}N_2O$
1,1-Diethylurea	$C_5H_{12}N_2O$
1,3-Diethylurea	$C_5H_{12}N_2O$
Diethyl zinc	$C_4H_{10}Zn$
Diethynyldiphenylgermane	$C_{16}H_{12}Ge$

1,1-Diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene	$C_{32}H_{22}Ge$
1,2-Difluorobenzene	$C_6H_4F_2$
1,3-Difluorobenzene	$C_6H_4F_2$
1,4-Difluorobenzene	$C_6H_4F_2$
4,4′-Difluorobiphenyl	$C_{12}H_8F_2$
1,1-Difluoroethane	$C_2H_4F_2$
Diformylhydrazine	$C_2H_4N_2O_2$
Diglycine nitrate	$C_4H_{11}N_3O_7$
Diglyme	$C_6H_{14}O_3$
4,4′-Diheptanoyloxydiphenyl-diacetylene	$C_{30}H_{34}O_4$
4,4′-Dihexanoyloxydiphenyl-diacetylene	$C_{28}H_{30}O_4$
Di-*n*-hexylammonium chloride	$C_{12}H_{28}ClN$
Di-*n*-hexyl sebacate	$C_{22}H_{42}O_4$
9,10-Dihydroanthracene	$C_{14}H_{12}$
4,5-Dihydro-2,3-benzofuran	C_8H_8O
2,5-Dihydrofuran clathrate hydrate	$C_4H_6O{\cdot}17H_2O$
9,10-Dihydrophenanthrene	$C_{14}H_{12}$
3,4-Dihydroxybenzaldehyde	$C_7H_6O_3$
1,2-Dihydroxybenzene	$C_6H_6O_2$
1,3-Dihydroxybenzene	$C_6H_6O_2$
1,4-Dihydroxybenzene	$C_6H_6O_2$
4,4′-Dihydroxybiphenyl	$C_{12}H_{10}O_2$
1,4-Dihydroxybutane	$C_4H_{10}O_2$
4,4′-Dihydroxydiphenyl-2,2-propane	$C_{15}H_{16}O_2$
1,2-Dihydroxyethane	$C_2H_6O_2$
1,5-Dihydroxy-3-oxapentane	$C_4H_{10}O_3$
1,2-Dihydroxypropane	$C_3H_8O_2$
3,5-Dihydroxytoluene monohydrate	$C_7H_8O_2{\cdot}H_2O$
1,2-Diiodobenzene	$C_6H_4I_2$
1,3-Diiodobenzene	$C_6H_4I_2$
1,4-Diiodobenzene	$C_6H_4I_2$
Diisobutyl amine	$C_8H_{19}N$
Diisobutyl ketone	$C_9H_{18}O$
1,6-Diisocyanatohexane	$C_8H_{12}N_2O_2$
1,1-Dimethylazoethane	$C_8N_{18}N_2$
1,1-Dimethylazoxyethane	$C_8H_{18}N_2O$
4,4′-Dimethoxyazoxybenzene	$C_{14}H_{14}N_2O_3$
1,1-Dimethoxy-3-cyanopropane	$C_6H_{11}NO_2$
2,2-Dimethoxypropane	$C_5H_{12}O_2$
Dimethyl acetal of β-cyanopropion-aldehyde	$C_6H_{11}NO_2$
Dimethylaminoethyl methacrylate	$C_8H_{15}NO_2$
3-Dimethylaminomethyl indole	$C_{11}H_{14}N_2$
Dimethylaminopropylenediamine	$C_5H_{15}N_3$
2,6-Dimethylaniline	$C_8H_{11}N$
1,2-Dimethylbenzene	C_8H_{10}
1,4-Dimethylbenzene	C_8H_{10}
2,2′-Dimethylbiphenyl	$C_{14}H_{14}$
2,2-Dimethylbutane	C_6H_{14}
2,3-Dimethylbutane	C_6H_{14}
3,3-Dimethyl-2-butanone	$C_6H_{12}O$
2,3-Dimethyl-2,3-bis(4-*tert*-butyl-phenyl)butane	$C_{26}H_{38}$
3,4-Dimethyl-3,4-bis(4-*tert*-butyl-phenyl)hexane	$C_{30}H_{46}$
1,4-Dimethylcubane dicarboxylate	$C_{12}H_{12}O_4$
2,3-Dimethyl-2,3-diphenylbutane	$C_{16}H_{18}$
N,N-Dimethylformamide	C_3H_7NO
2,6-Dimethyl-4-heptanone	$C_9H_{18}O$
N,N′-Dimethylhydrazine	$C_2H_8N_2$
N,N-Dimethylmethanamide	C_3H_7NO
2,3-Dimethylnaphthalene	$C_{12}H_{12}$
3,7-Dimethyl-6-octen-1-yn-3-ol	$C_{10}H_{16}O$
3,3-Dimethyl-2-oxabutane	$C_5H_{12}O$
3,4-Dimethylpentanal	$C_7H_{14}O$
2,3-Dimethylpentane	C_7H_{16}
3,3-Dimethylpentane	C_7H_{16}
N,N-Dimethyl-2-pentylnonylamine	$C_{16}H_{35}N$
2,3-Dimethylphenol	$C_8H_{10}O$
2,4-Dimethylphenol	$C_8H_{10}O$
2,5-Dimethylphenol	$C_8H_{10}O$
2,6-Dimethylphenol	$C_8H_{10}O$
3,4-Dimethylphenol	$C_8H_{10}O$
3,5-Dimethylphenol	$C_8H_{10}O$
3,4-Dimethylphospholyl manganese tricarbonyl	$C_9H_8MnO_3P$
Dimethyl *o*-phthalate	$C_{10}H_{10}O_4$
N,N-Dimethyl-1,3-propanediamine	$C_5H_{14}N_2$
2,2-Dimethylpropanamide	$C_5H_{11}NO$
2-(1,2-Dimethylpropyl)-5,6-methylheptenal	$C_{14}H_{26}O$
2,3-Dimethylpyridine	C_7H_9N
2,4-Dimethylpyridine	C_7H_9N
2,5-Dimethylpyridine	C_7H_9N
2,6-Dimethylpyridine	C_7H_9N
3,4-Dimethylpyridine	C_7H_9N
3,5-Dimethylpyridine	C_7H_9N
2,4-Dimethylpyrrole	C_6H_9N
2,5-Dimethylpyrrole	C_6H_9N
1,1-Dimethyl-1-silacyclobutane	$C_5H_{12}Si$
6,10-Dimethyl-2-undecanone	$C_{13}H_{26}O$
6,10-Dimethyl-4,5,9-undecatrien-2-one	$C_{13}H_{20}O$
6,10-Dimethyl-3,5,9-undecatrien-2-one	$C_{13}H_{20}O$
1,3-Dimethyluracil	$C_6H_8N_2O_2$
1,1-Dimethylurea	$C_3H_8N_2O$
1,3-Dimethylurea	$C_3H_8N_2O$
Dimethylzinc	C_2H_6Zn
Dinitrile-2,2′-azodiisobutyric acid	$C_8H_{12}N_4$
1,2-Dinitrobenzene	$C_6H_4N_2O_4$
1,3-Dinitrobenzene	$C_6H_4N_2O_4$
1,4-Dinitrobenzene	$C_6H_4N_2O_4$
2,3-Dinitrophenol	$C_6H_4N_2O_5$
2,4-Dinitrophenol	$C_6H_4N_2O_5$
2,5-Dinitrophenol	$C_6H_4N_2O_5$
2,6-Dinitrophenol	$C_6H_4N_2O_5$
3,4-Dinitrophenol	$C_6H_4N_2O_5$
3,5-Dinitrophenol	$C_6H_4N_2O_5$
2,2-Dinitropropane	$C_3H_6N_2O_4$
4,4′-Dinonanoyloxydiphenyl diacetylene	$C_{34}H_{42}O_4$
4,4′-Dioctanoyloxydiphenyl-diacetylene	$C_{32}H_{38}O_4$
Di-*n*-octylammonium chloride	$C_{16}H_{36}ClN$
Dioctyl *o*-phthalate	$C_{24}H_{38}O_4$
1,4-Dioxane	$C_4H_8O_2$
1,3-Dioxane clathrate hydrate	$C_4H_8O_2{\cdot}17H_2O$
1,4-Dioxane-2,5-dione	$C_4H_4O_4$
3,6-Dioxaoctane	$C_6H_{10}O_2$
1,3-Dioxolan	$C_3H_6O_2$
1,3-Dioxolane clathrate hydrate	$C_3H_6O_2{\cdot}17H_2O$
2,5-Dioxopiperazine	$C_4H_6N_2O_2$
4,4′-Dipentanoyloxydiphenyldiacetylene	$C_{26}H_{26}O_4$
Di-*n*-pentylammonium chloride	$C_{10}H_{24}ClN$
Diphenyl	$C_{12}H_{10}$
Diphenylacetylene	$C_{14}H_{10}$
1,2-Diphenylbenzimidazole	$C_{19}H_{14}N_2$
1,1′-Diphenyl-1,1′-bicyclohexane	$C_{24}H_{30}$
1,1′-Diphenyl-1,1′-bicyclooctane	$C_{26}H_{34}$
1,1′-Diphenyl-1,1′-bicyclopentane	$C_{22}H_{26}$
Diphenylcarbodiimide	$C_{13}H_{10}N_2$
Diphenyldiethynylsilane	$C_{16}H_{12}Si$
Diphenyl diketone	$C_{14}H_{10}O_2$
1,1-Diphenyldodecane	$C_{24}H_{34}$
4′,4″-Diphenylenephthalidodicarboxylic acid dihydrazide	$C_{22}H_{18}N_4O_4$
1,2-Diphenylethane	$C_{14}H_{14}$
Diphenylethyne	$C_{14}H_{10}$

Diphenylmethane	$C_{13}H_{12}$
4,4′-Diphenyl methane diisocyanate	$C_{15}H_{10}N_2O_2$
1,3-Diphenylurea	$C_{13}H_{12}N_2O$
Dipiperazinylethane	$C_{10}H_{22}N_4$
4,4′-Dipropanoyloxydiphenyldiacetylene	$C_{22}H_{18}O_4$
Dipropylamine	$C_6H_{15}N$
4,5-Dipropyl-4,5-bis(4-*tert*-butylphenyl)octane	$C_{34}H_{54}$
Dipropylene glycol	$C_6H_{14}O_3$
1,3-Dithiane	$C_4H_8S_2$
1,4-Dithiane	$C_4H_8S_2$
4,4′-Diundecanoyloxydiphenyldiacetylene	$C_{38}H_{50}O_4$
n-Docosane	$C_{22}H_{46}$
n-Dodecane	$C_{12}H_{26}$
1-Dodecanethiol	$C_{12}H_{28}S$
n-Dodecyl mercaptan	$C_{12}H_{28}S$
Dodecylammonium tetrachloromanganate	$C_{24}H_{56}N_2MnCl_4$
Dodecylammonium tetrachloromanganate (II)	$C_{24}H_{56}Cl_4MnN_2$
Dodecylammonium tetrachlorozincate (II)	$C_{24}H_{56}Cl_4N_2Zn$
n-Dotriacontane	$C_{32}H_{66}$
Dulcite	$C_6H_{14}O_6$
Dulcitol	$C_6H_{14}O_6$

E

n-Eicosane	$C_{20}H_{42}$
1-Eicosanethiol	$C_{20}H_{42}S$
n-Eicosanyl mercaptan	$C_{20}H_{42}S$
Enanthal	$C_7H_{14}O$
ζ-Enantholactam	$C_7H_{13}NO$
Endobicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid anhydride	$C_9H_8O_3$
Ethanal	C_2H_4O
Ethanamide	C_2H_5NO
Ethane	C_2H_6
1,2-Ethanediol	$C_2H_6O_2$
Ethanoic acid	$C_2H_4O_2$
N-Ethanol isatoxine	$C_{10}H_{10}N_2O_2$
Ethanol	C_2H_6O
4-Ethoxy-4′-butylazobenzene	$C_{18}H_{22}N_2O$
N-*p*-Ethoxybenzylidene-*p*′-butylaniline	$C_{19}H_{23}NO$
2-Ethoxyethanol acetate	$C_6H_{12}O_3$
2-Ethoxyisonitrosoacetanilide	$C_{10}H_{12}N_2O_3$
4-Ethoxyisonitrosoacetanilide	$C_{10}H_{12}N_2O_3$
Ethyl acetate	$C_4H_8O_2$
Ethyl alcohol	C_2H_6O
2-Ethylbiphenyl	$C_{14}H_{14}$
Ethyl carbamate	$C_3H_7NO_2$
Ethyl cyanoacetate	$C_5H_7NO_2$
Ethyl-2,2-dimethylpropanoate	$C_7H_{14}O_2$
Ethyl ethanoate	$C_4H_8O_2$
2-Ethylhexanol	$C_8H_{18}O$
Ethyl phenyl ether	$C_8H_{10}O$
Ethyl propanoate	$C_5H_{10}O_2$
Ethyl propionate	$C_5H_{10}O_2$
Ethyl *n*-propyl ether	$C_5H_{12}O$
Ethyl urea	$C_3H_8N_2O$
Ethylene	C_2H_4
Ethylene butadiene copolymer	$(C_6H_{10})_n$
Ethylenediamine	$C_2H_8N_2$
Ethylene dibromide	$C_2H_4Br_2$
Ethylene dichloride	$C_2H_4Cl_2$
Ethylene glycol	$C_2H_6O_2$
Ethylene glycol acetate	$C_4H_8O_3$
Ethylene glycol diacetate	$C_6H_{10}O_4$
Ethylene glycol dipropanoate	$C_8H_{14}O_4$
Ethylene glycol dibutanoate	$C_{10}H_{18}O_4$
Ethylene oxalate	$C_4H_4O_4$
Ethylene oxide hydrate	$C_2H_4O{\cdot}7H_2O$
Ethylidene difluoride	$C_2H_4F_2$
Eugenol	$C_{10}H_{12}O_2$

F

Ferrocene	$C_{10}H_{10}Fe$
Ferrocene-d_{10}	$C_{10}D_{10}Fe$
Ferrocene-d_{10} thiourea clathrate(1:3)	$C_{13}H_{12}D_{10}FeN_6S_3$
Ferrocenium hexafluorophosphate	$C_{10}H_{10}F_6FeP$
Fluoranthene picric acid	$C_{22}H_{13}N_3O_7$
Fluorene picric acid	$C_{19}H_{13}N_3O_7$
Fluorobenzene	C_6H_5F
2-Fluoronaphthalene	$C_{10}H_7F$
4-Fluorotoluene	C_7H_7F
Fluorotrichloromethane	CCl_3F
Formamide	CH_3NO
Freon 11	CCl_3F
Freon 14	CF_4
Freon 113	$C_2Cl_3F_3$
Freon 152A	$C_2H_4F_2$
Freon C318	C_4F_8
Fructose	$C_6H_{12}O_6$
Fructose(D)	$C_6H_{12}O_6$

G

Galactitol	$C_6H_{14}O_6$
Galactose(D)	$C_6H_{12}O_6$
Gallium triethyl	$C_6H_{15}Ga$
Galvinoxyl hydrogalvinoxyl (6:1) radical	$C_{203}H_{288}O_{14}$
Galvinoxyl hydrogalvinoxyl (9:1) radical	$C_{290}H_{411}O_{20}$
Geranial	$C_{10}H_{16}O$
α-Glucose(D)	$C_6H_{12}O_6$
Glutamic acid	$C_5H_9NO_4$
Glycerol	$C_3H_8O_3$
Glycerol triacetate	$C_9H_{14}O_6$
Glyceryl tributyrate	$C_{15}H_{26}O_6$
Glyceryl trimargarate	$C_{54}H_{104}O_6$
Glyceryl tristearate	$C_{57}H_{110}O_6$
Glycolide	$C_4H_4O_4$
Gramine	$C_{11}H_{14}N_2$
Graphite	C

H

n-Henicosane	$C_{21}H_{44}$
n-Heptacosane	$C_{27}H_{56}$
n-Heptadecane	$C_{17}H_{36}$
n-Heptaldehyde	$C_7H_{14}O$
2,2,4,4,6,8,8-Heptamethylnonane	$C_{16}H_{34}$
1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane	$C_{11}H_{20}O_3Si_3$
Heptanal	$C_7H_{14}O$
n-Heptane	C_7H_{16}
Heptanol	$C_7H_{16}O$
1-Heptanol	$C_7H_{16}O$
4-*n*-Heptoxyphenyl-4′-*n*-butylbenzoate	$C_{24}H_{32}O_3$
n-Heptyl alcohol	$C_7H_{16}O$
Hexachloroethane	C_2Cl_6
n-Hexacosane	$C_{26}H_{54}$
Hexadecafluoroheptane	C_7F_{16}
n-Hexadecane	$C_{16}H_{34}$
1-Hexadecanethiol	$C_{16}H_{34}S$
1-Hexadecanol	$C_{16}H_{34}O$
n-Hexadecyl mercaptan	$C_{16}H_{34}S$
2,4-Hexadiyne	C_6H_6
Hexa-O-decanoyl-scyllo-inositol	$C_{66}H_{120}O_{12}$
Hexaethylbenzene	$C_{18}H_{30}$
1,1,3,3,5,5-Hexaethylcyclotrisiloxane	$C_{12}H_{30}O_3Si_3$
Hexaethylene glycol	$C_{12}H_{26}O_7$
Hexafluorobenzene	C_6F_6
Hexa-O-hexanoyl-scyllo-inositol	$C_{42}H_{72}O_{12}$

Hexahydroxyhexaethylenediamine chromium sulfate decahydrate	$C_{12}H_{52}Cr_4N_{12}O_{18}S_3 \cdot 10H_2O$
Hexamethyldisilane	$C_6H_{18}Si_2$
1,6-Hexamethylene diisocyanate	$C_8H_{12}N_2O_2$
1,6-Hexamethylene diisocyanate polycyclotrimer	$(C_8H_{12}N_2O_2)_n$
1-Hexanol	$C_6H_{14}O$
2,3,6,7,10,11-Hexa-*n*-octanoyloxy-triphenylene	$C_{66}H_{96}O_{12}$
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid I)	$C_{66}H_{96}O_{12}$
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid II)	$C_{66}H_{96}O_{12}$
2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene (solid III)	$C_{66}H_{96}O_{12}$
Hexa-O-octanoyl-scyllo-inositol	$C_{54}H_{96}O_{12}$
4bα,4cβ,5,9bβ,9cα,10-Hexahydrocyclabuta[1,2-a:3,4-a']diindene	$C_{18}H_{16}$
4bβ,4cα,9,9aα,9bβ,10-Hexahydrocyclobuta[1,2-a:4,3-a']diindene	$C_{18}H_{16}$
1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane	$C_9H_{24}Si_3$
1,1,1,5,5,5-Hexamethyl-3,3-diphenyltrisiloxane	$C_{24}H_{28}O_2Si_3$
1,1,3,3,5,5-Hexamethyl-7,7-diphenyltetrasiloxane	$C_{18}H_{28}Si_4O_4$
Hexamethylbenzene	$C_{12}H_{18}$
Hexamethyldisilylmethane	$C_7H_{20}Si_2$
1,6-Hexamethylene diisocyanate	$C_8H_{12}N_2$
Hexamethylphosphoramide	$C_6H_{18}N_3OP$
Hexamethylphosphoric triamide	$C_6H_{18}N_3OP$
cis-(5,12)-7,7,14,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane	$C_{16}H_{36}N_4$
Hexamethyltrisilazane	$C_6H_{21}N_3Si_3$
n-Hexane	C_6H_{14}
1,6-Hexanediol	$C_6H_{14}O_2$
1-Hexanethiol	$C_6H_{14}S$
1-Hexanol	$C_6H_{14}O$
2-Hexanone	$C_6H_{12}O$
3-Hexanone	$C_6H_{12}O$
1,1,3,3,5,5-Hexaphenyl-7,7-dimethyl-cyclotetrasiloxane	$C_{38}H_{36}O_4Si_4$
Hexaphenylisomelamine	$C_{39}H_{30}N_6$
Hexaphenylmelamine	$C_{39}H_{30}N_6$
Hexapropylene glycol	$C_{18}H_{38}O_7$
n-Hexatriacontane	$C_{36}H_{74}$
1-Hexene	C_6H_{12}
n-Hexyl alcohol	$C_6H_{14}O$
n-Hexyl ethanoate	$C_8H_{16}O_2$
n-Hexyl mercaptan	$C_6H_{14}S$
p-*n*-Hexyloxybenzylideneaniline	$C_{19}H_{23}NO$
p-*n*-Hexyloxybenzylideneamino-*p'*-benzonitrile	$C_{20}H_{22}N_2O$
p-*n*-Hexyloxybenzylideneamino-*p'*-chlorobenzene	$C_{19}H_{22}ClNO$
p-*n*-Hexyloxybenzylideneamino-*p'*-fluorobenzene	$C_{19}H_{22}FNO$
N-*p*-*n*-Hexyloxybenzylidene-*p'*-*n*-butylaniline	$C_{23}H_{31}NO$
p-*n*-Hexyloxybenzylidene-*p'*-toluidine	$C_{20}H_{25}NO$
1-Hexynylcopper	C_6H_9Cu
HMX	$C_4H_8N_8O_8$
Homocubane-4-carboxylic acid	$C_{10}H_{10}O_2$
Hydrazinium hydrogen oxalate	$C_2H_6N_2O_4$
Hydroquinone	$C_6H_6O_2$
1-Hydroxyadamantane	$C_{10}H_{16}O$
2-Hydroxyadamantane	$C_{10}H_{16}O$
2-(2'-Hydroxyethoxy)ethyl pivalate	$C_9H_{18}O_4$
2-Hydroxyethyl-2',2'-dimethyl-propionate	$C_7H_{14}O_3$
2-Hydroxyethyl pivalate	$C_7H_{14}O_3$
2-Hydroxypropanoic acid (DL)	$C_3H_6O_3$
m-Hydroxytoluene	C_7H_8O
o-Hydroxytoluene	C_7H_8O
p-Hydroxytoluene	C_7H_8O

I

Imidazole	$C_3H_4N_2$
Indazole	$C_7H_6N_2$
Indene picric acid	$C_{15}H_{11}N_3O_7$
3-Indole aldehyde	C_9H_7NO
Indole	C_8H_7N
meso-Inositol	$C_6H_{12}O_6$
Iodobis(N,N-dimethyldithiocarbamato) iron (III)	$C_6H_{12}FeIN_2S_4$
Iodomethane	CH_3I
Iron (III) acetylacetonate	$C_{15}H_{21}FeO_6$
Isoamyl propionate	$C_8H_{16}O_2$
Isobutene	C_4H_8
Isobutyl alcohol	$C_4H_{10}O$
Isobutylmethylketone	$C_6H_{12}O$
Isobutyric acid	$C_4H_8O_2$
Isochroman	C_9H_7O
1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene	$C_{13}H_{15}NO$
1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene	$C_{13}H_{15}NO$
Isonitrosoacetanilide	$C_8H_8N_2O_2$
Isooctane	C_8H_{18}
Isooctyl alcohol	$C_8H_{18}O$
Isophytol	$C_{20}H_{40}O$
Isopropyl methyl ketone	$C_5H_{10}O$
Isopropyl nitrate	$C_3H_7NO_3$
Isopropyl urea	$C_4H_{10}N_2O$
Isoquinoline	C_9H_7N

L

Lactic acid (DL)	$C_3H_6O_3$
Lactide (DL)	$C_6H_8O_4$
Lactose, anhydrous	$C_{12}H_{22}O_{11}$
Lead dicalcium propionate	$C_{18}H_{30}Ca_2O_{12}Pb$
Leucine (L)	$C_6H_{13}NO_2$
Lithium acetate dihydrate	$C_2H_3LiO_2 \cdot 2H_2O$
Lithium butyrate	$C_4H_7LiO_2$
Lithium n-heptanoate	$C_7H_{13}LiO_2$
Lithium n-hexanoate	$C_6H_{11}LiO_2$
Lithium n-pentanoate	$C_5H_9LiO_2$
Lithium propionate	$C_3H_5LiO_2$

M

Magnesium acetate	$C_4H_6O_4Mg$
Magnesium diethanoate tetrahydrate	$C_4H_6MgO_4 \cdot 4H_2O$
Malononitrile	$C_3H_2N_2$
Maleic anhydride	$C_4H_2O_3$
Maltose	$C_{12}H_{22}O_{11}$
Manganocene	$C_{10}H_{10}Mn$
Mannitol	$C_6H_{14}O_6$
Mannitol(D)	$C_6H_{14}O_6$
Mannose(D)	$C_6H_{12}O_6$
Manxane	$C_{11}H_{20}$
Methacrylic acid	$C_4H_6O_2$
p-Methacryloyloxybenzoic acid	$C_{11}H_{10}O_4$
Methanamide	CH_3NO
Methane	CH_4
Methanol	CH_4O
Methionine (DL)	$C_5H_{11}NO_2S$
Methionine (L)	$C_5H_{11}NO_2S$
Methoxybenzene	C_7H_8O
N-(4-Methoxybenzylidene)-*p*-(*n*-butyl)-aniline	$C_{18}H_{21}NO$
2-Methoxyethanol acetate	$C_5H_{10}O_3$
2-Methoxyisonitrosoacetanilide	$C_9H_{10}N_2O_3$

4-Methoxyisonitrosoacetanilide	$C_9H_{10}N_2O_3$
2-Methoxy-1-propene	C_4H_8O
3-Methoxypropylamine	$C_4H_{11}NO$
Methyl acrylate	$C_4H_6O_2$
α-Methyl acrylic acid	$C_4H_6O_2$
Methyl alcohol	CH_4O
Methylammonium hexachloro-tellurate	$C_2H_{12}Cl_6Te$
Methylammonium iodide	CH_6IN
4-Methylaniline	C_7H_9N
N-Methylaniline	C_7H_9N
2-Methyl-2-butanol	$C_5H_{12}O$
3-Methyl-2-butanone	$C_5H_{10}O$
2-Methyl-1-butene	C_5H_{10}
2-Methyl-2-butene	C_5H_{10}
3-Methyl-1-butene	C_5H_{10}
2-Methyl-3-buten-2-ol	$C_5H_{10}O$
4-(2-Methylbutoxy)phenyl ester of 4-*n*-decycloxybenzoic acid (D)	$C_{28}H_{40}O_4$
Methyl *n*-butyl ether	$C_5H_{12}O$
Methyl *tert*-butyl ether	$C_5H_{12}O$
Methyl carbamate	$C_2H_5NO_2$
N-Methylcarbazole	$C_{13}H_{11}N$
Methylchloroform	$C_2H_3Cl_3$
Methyl cyanide	C_2H_3N
Methylcyclohexane	C_7H_{14}
4-Methylcyclohexene	C_7H_{12}
Methyl *n*-decyl ether	$C_{11}H_{24}O$
3,3'-Methylene bis(6-aminophenol)	$C_{13}H_{14}N_2O_2$
Methylenecyclobutane	C_5H_8
Methylene dichloride	CH_2Cl_2
Methylene glycol acetate	$C_3H_6O_3$
Methyl ester of nitroacetic acid	$C_3H_5NO_4$
Methylethylethanolamine	$C_5H_{13}NO$
Methyl ethyl ketone	C_4H_8O
N-Methylformamide	C_2H_5NO
Methyl formate	$C_2H_4O_2$
2-Methyl-1-heptanol	$C_8H_{18}O$
6-Methyl-5-hepten-2-one	$C_8H_{14}O$
3-Methylhexanal	$C_7H_{14}O$
Methyl iodide	CH_3I
Methyl methacrylate	$C_5H_8O_2$
N-Methylmethanamide	C_2H_5NO
Methyl methanoate	$C_2H_4O_2$
Methyl 2-methylpropenoate	$C_5H_8O_2$
Methyl nitroacetate	$C_3H_5NO_4$
2-Methyloxirane	C_3H_6O
N-Methylpentanamide	$C_6H_{13}NO$
2-Methylpentane	C_6H_{14}
3-Methylpentane	C_6H_{14}
2-Methyl-1-pentanol	$C_6H_{14}O$
3-Methyl-2-pentanol	$C_6H_{14}O$
3-Methyl-3-pentanol	$C_6H_{14}O$
4-Methyl-2-pentanol	$C_6H_{14}O$
4-Methyl-2-pentanone	$C_6H_{12}O$
Methyl perfluorobutanoate	$C_5H_3F_7O_2$
4-Methylphenanthrene	$C_{15}H_{12}$
2-Methylphenol	C_7H_8O
3-Methylphenol	C_7H_8O
4-Methylphenol	C_7H_8O
2-Methylpiperidine	$C_6H_{13}N$
Methyl phenyl ether	C_7H_8O
2-Methylpropanamide	C_4H_9NO
Methyl propanoate	$C_4H_8O_2$
2-Methylpropanoic acid	$C_4H_8O_2$
2-Methyl-1-propanol	$C_4H_{10}O$
2-Methyl-2-propanol	$C_4H_{10}O$
2-Methylpropene	C_4H_8
Methyl propenoate	$C_4H_6O_2$
Methyl propionate	$C_4H_8O_2$
Methyl *n*-propyl ether	$C_4H_{10}O$
2-Methylpyridine	C_6H_7N
4-Methylpyridine	C_6H_7N
N-Methylpyrrole	C_5H_7N
3-Methylpyrrolidine	$C_5H_{11}N$
Methyl silicate	$C_4H_{12}O_4Si$
α-Methylstyrene	C_9H_{10}
Methyl trichlorothioacrylate	$C_4H_3Cl_3OS$
Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodimethanide)	$C_{43}H_{26}N_8P$
N-Methylvaleramide	$C_6H_{13}NO$
4-Methyoxy-4'-heptanoylazobenzene	$C_{20}H_{24}N_2O_3$
Milk sugar	$C_{12}H_{22}O_{11}$
Mixed valence iron oxo-centered complex with acetate and 3-methyl pyridine	$C_{36}H_{46}Fe_3N_4O_{13}$
Monobutylurea	$C_5H_{12}N_2O$
Mono-*tert*-butylurea	$C_5H_{12}N_2O$
Monochloroacetic acid	$C_2H_3ClO_2$
Monoethylurea	$C_3H_8N_2O$
Monoisopropylurea	$C_4H_{10}N_2O$
Monomethylurea	$C_2H_6N_2O$
Monophenylurea	$C_7H_8N_2O$
Monopropylurea	$C_4H_{10}N_2O$
Morpholine	C_4H_9NO

N

Naphthalene picric acid	$C_{16}H_{11}N_3O_7$
Naphthalene-tetracyanobenzene	$C_{20}H_{10}N_4$
Naphthalene-tetracyanoethylene	$C_{18}H_8N_4$
Naphthalene	$C_{10}H_8$
Natural ricinoleic acid	$C_{18}H_{34}O_3$
Nickelocene	$C_{10}H_{10}Ni$
3-Nitroaniline	$C_6H_6N_2O_2$
4-Nitroaniline	$C_6H_6N_2O_2$
p-Nitroanisole	$C_7H_7NO_3$
Nitrobenzene	$C_6H_5NO_2$
4-Nitrobenzoic acid	$C_7H_6NO_2$
4-Nitrochlorobenzene	$C_6H_4ClNO_2$
p-Nitroethoxybenzene	$C_8H_9NO_3$
4-Nitromethoxybenzene	$C_7H_7NO_3$
p-Nitrophenetole	$C_8H_9NO_3$
2-Nitrophenol	$C_6H_5NO_3$
3-Nitrophenol	$C_6H_5NO_3$
4-Nitrophenol	$C_6H_5NO_3$
4'-Nitrophenyl-4-*n*-octyloxybenzoate	$C_{21}H_{25}NO_5$
4-Nitrophenyl-4'-octyloxybenzoate	$C_{21}H_{25}NO_5$
n-Nonacosane	$C_{29}H_{60}$
n-Nonadecane	$C_{19}H_{40}$
Nonanal	$C_9H_{18}O$
n-Nonane	C_9H_{20}
5-Nonanone	$C_9H_{18}O$
Nonylcyanobiphenyl	$C_{22}H_{27}N$
Nonyl methacrylate	$C_{13}H_{24}O_2$
Norbornadiene	C_7H_8
Norbornane	C_7H_{12}
Norbornene	C_7H_{10}
Norleucine (DL)	$C_6H_{13}NO_2$
Norleucine (L)	$C_6H_{13}NO_2$
Northindrone 4-cyclohexylbenzoate	$C_{33}H_{40}O_2$
Northindrone-6-(4-chlorophenyl)-hexanoate	$C_{32}H_{39}ClO_2$
Northindrone acetate	$C_{22}H_{28}O_2$
Northindrone benzoate	$C_{27}H_{30}O_2$
Northindrone biphenyl-4-carboxylate	$C_{33}H_{34}O_2$
Northindrone dimethylpropionate	$C_{25}H_{34}O_2$
Northindrone heptanoate	$C_{27}H_{38}O_2$
Northindrone pentamethyldisiloxyl ether	$C_{25}H_{40}O_2Si_2$
Northindrone *trans*-3-(4-butylcyclo-hexyl)propionate	$C_{33}H_{48}O_2$
Northindrone *trans*-4-hexylcyclo-hexylcarboxylate	$C_{33}H_{34}O_2$

Northindrone	$C_{20}H_{26}O$
Nortricyclene	C_7H_{10}
Norvaline (L)	$C_5H_{11}NO_2$

O

n-Octacosane	$C_{28}H_{58}$
n-Octadecane	$C_{18}H_{38}$
1-Octadecanethiol	$C_{18}H_{38}S$
Octadecanoic acid	$C_{18}H_{36}O_2$
Octadecylammonium cadmium tetrachloride	$C_{36}H_{80}CdCl_4N_2$
n-Octadecyl mercaptan	$C_{18}H_{38}S$
Octaethylcyclotetrasiloxane	$C_{16}H_{40}O_4Si_4$
Octafluorocyclobutane	C_4F_8
Octagen	$C_4H_8N_8O_8$
Octagen(α)	$C_4H_8N_8O_8$
Octagen(β)	$C_4H_8N_8O_8$
1,2,3,4,5,6,7,8-Octahydroanthracene	$C_{14}H_{18}$
5,6,6a,6b,7,8,12b,12c-Octahydrodibenzo[a,i]biphenylene	$C_{20}H_{20}$
5,6,6a,6b,11,12,12a,12b-Octahydrodibenzo[a,g]biphenylene	$C_{20}H_{20}$
1,1,4,4,10,10,13,13-Octamethylcyclooctadecane	$C_{26}H_{52}$
Octamethyltetrasiloxane	$C_8H_{24}Si_4O_4$
Octamethyltetrasilazane	$C_8H_{28}Ni_4Si$
Octanal	$C_8H_{16}O$
n-Octane	C_8H_{18}
1-Octanethiol	$C_8H_{16}S$
Octanol	$C_8H_{18}O$
1-Octanol	$C_8H_{18}O$
Octaphenylcyclotetrasiloxane	$C_{48}H_{40}O_4Si_4$
Octa(vinylsilasesquioxane)	$C_{16}H_{24}Si_8O_{12}$
4-Octyl-4′-heptyl-α-cyanostilbene	$C_{20}H_{41}NO$
n-Octyl alcohol	$C_8H_{18}O$
n-Octyl mercaptan	$C_8H_{16}S$
n-Octyl methacrylate	$C_{12}H_{22}O_2$
Octylcyanobiphenyl	$C_{21}H_{25}N$
Oenanthal	$C_7H_{14}O$
Oligoethylene butylene glycol adipate	$C_{12}H_{22}O_6$
Orcinol monohydrate	$C_7H_8O_2{\cdot}H_2O$
2-Oxadodecane	$C_{11}H_{24}O$
2-Oxahexane	$C_5H_{12}O$
3-Oxahexane	$C_5H_{12}O$
Oxalyl fluoride	$C_2F_2O_2$
2-Oxapentane	$C_4H_{10}O$
Oxolane	C_4H_8O
μ_3-Oxo-tris(pyridine)hexakis(acetato) iron(II)-diiron monopyridine	$C_{32}H_{38}Fe_3N_4O_{15}$

P

2,2-Paracyclophane	$C_{16}H_{16}$
Pelargonaldehyde	$C_9H_{18}O$
n-Pentacosane	$C_{25}H_{52}$
n-Pentadecane	$C_{15}H_{32}$
Pentaerythritol	$C_5H_{12}O_4$
2,2,4,6,6-Pentamethylheptane	$C_{12}H_{26}$
n-Pentanal	$C_5H_{10}O$
1-Pentanol	$C_5H_{12}O$
tert-Pentanol	$C_5H_{12}O$
2-Pentanone	$C_5H_{10}O$
3-Pentanone	$C_5H_{10}O$
Pentapropylene glycol	$C_{15}H_{32}O_6$
1-Pentene	C_5H_{10}
cis-2-Pentene	C_5H_{10}
trans-2-Pentene	C_5H_{10}
n-Pentyl alcohol	$C_5H_{12}O$
tert-Pentyl alcohol	$C_5H_{12}O$
Pentyl butanoate	$C_9H_{18}O_2$
Pentyl propionate	$C_8H_{16}O_2$
n-Pentylamine	$C_5H_{13}N$
Pentyldiamine manganese tetrachloride	$C_5H_{16}Cl_4Mn$
2-Pentylnonenal	$C_{14}H_{26}O$
N-*p*-*n*-Pentyloxybenzylidene-*p*′-*n*-butylaniline	$C_{22}H_{29}NO$
Perchlorobiphenyl	$C_{12}Cl_{10}$
Perfluorobenzene	C_6F_6
Perfluorobiphenyl	$C_{12}F_{10}$
n-Perfluorobutane	C_4F_{10}
Perfluoroheptane	C_7F_{16}
n-Perfluorohexane	C_6F_{14}
Perfluoromethyldiethylamine	$C_5F_{13}N$
n-Perfluoropentane	C_5F_{12}
Perfluorotriethylamine	$C_6F_{15}N$
Perhydrophenanthrene	$C_{14}H_{24}$
Perylene picric acid	$C_{26}H_{15}N_3O_7$
Phenanthrene	$C_{14}H_{10}$
Phenanthridine	$C_{13}H_9N$
Phenol	C_6H_6O
Phenolphthalein	$C_{20}H_{14}O_4$
1-Phenyl-1-cyclohexyldodecane	$C_{24}H_4O$
Phenyl glycidyl ether	$C_9H_{10}O_2$
Phenylacetylene	C_8H_6
Phenylaminoethyl methacrylate	$C_{12}H_{15}NO_2$
1,3-Phenylenediamine	$C_6H_8N_2$
Phenylhydrazine	$C_6H_8N_2$
3-Phenyl-5-phenoxymethyl-2-N-phenyliminooxazolidine	$C_{22}H_{20}N_2O_2$
3-Phenyl-5-phenoxymethyl-2-oxazolidinone	$C_{16}H_{15}NO_3$
N-Phenylphthalimide	$C_{14}H_{11}NO_3$
Phenylpropionic acid	$C_9H_{10}O_2$
o-Phenylenepyrene picric acid	$C_{28}H_{15}N_3O_7$
Phenyltrichlorogermane	$C_6H_5Cl_3Ge$
Phenyltrichlorostannane	$C_6H_5Cl_3Sn$
Phenyl-*o*-tolylmethane	$C_{14}H_{14}$
Phenylurea	$C_7H_8N_2O$
Phosphaferrocene	C_9H_9FeP
Phthalanilic acid	$C_{14}H_9NO_2$
Phthalic anhydride	$C_8H_4O_3$
Phthalonitrile and *m*-phenylene diamine condensation product	$C_{28}H_{18}N_6$
o-Phthalonitrile	$C_8H_4N_2$
Phytone	$C_{18}H_{36}O$
Picene picric acid	$C_{28}H_{17}N_3O_7$
α-Picoline	C_6H_7N
Picric acid	$C_6H_3N_3O_7$
Piperazine	$C_4H_{10}N_2$
Piperidine	$C_5H_{11}N$
α-Piperidone	C_5H_9NO
Pival aldehyde	$C_5H_{10}O$
Polyacetylene	$(CH)_n$
Polybenzimidazoloquinazole	$(C_{34}H_{18}N_6O)_n$
Poly(2,2-bis-(4-phenoxypropane) 2,4,6-triazine	$(C_{17}H_{14}N_2)_n$
cis-1,4-Polybutadiene	$(C_4H_6)n$
trans-1,4-Polybutadiene	$(C_4H_6)n$
Polybutylene glycol adipate	$(C_{10}H_{16}O_4)_n$
Poly(butylene terephthalate)	$(C_{12}H_{12}O_4)_n$
Poly-ϵ-caprolactam	$(C_6H_{11}NO)_n$
Poly-ϵ-caprolactone	$(C_6H_{10}O_2)_n$
Polycyanate	$(C_{17}H_{14}N_2O_2)_n$
Poly(diethylsiloxane)	$(C_4H_{10}OSi)_n$
Poly-1,1-diethynyl-2,3,4,5-tetraphenyl-1-germacyclopentadiene	$(C_{32}H_{22}Ge)_n$
Poly-4,4′-dihydroxy-3,3′-isophthalamidodiphenylmethane	$(C_{21}H_{16}N_2O_4)_n$
Poly(dimethylsiloxane)	$(C_2H_6OSi)_n$
Poly-1,3-dioxolan	$(C_3H_6O_2)_n$
Polydiphenyldiethynylgermanium	$(C_{16}H_{10}Ge)_n$

Polydiphenyldiethynylgermanium	$(C_{16}H_{10}Ge)_n$
Poly(*p,p'*-diphenylene oxide) pyromellitimide	$C_{22}H_{14}N_2O_7$
Poly(*p,p'*-diphenylenephthalido)hydrazide	$(C_{30}H_{20}N_4O_6)_n$
Poly(*p,p'*-diphenylenephthalido)-1,3,4-oxadiazole	$(C_{30}H_{16}N_4O_4)_n$
Polyethylene	$(CH_2)_n$
Polyethylene glycol	$(C_2H_4O)_n$
Polyethylene oxalate	$(C_4H_4O_4)_n$
Polyglycine I	$(C_2H_3NO)_n$
Polyglycine II	$(C_2H_3NO)_n$
Polyglycolide	$(C_4H_4O_4)_n$
Poly(hexamethylene sebacate)	$(C_{38}H_{70}O_8)_n$
1-Polyhexene	$(C_6H_{12})_n$
Polyisobutylene	$(C_4H_8)_n$
Polyisocyanurate	$(C_{15}H_{10}N_2O_2)_n$
Polymethacrylic acid	$(C_4H_6O_2)_n$
Poly-*p*-methyacryloyloxybenzoic acid	$(C_{11}H_{10}O_4)_n$
Poly(methyl methacrylate)	$(C_5H_8O_2)_n$
Poly(α-methylstyrene)	$(C_9H_{10})_n$
Polyoctenylene	$(C_8H_{14})_n$
Polypentenamer	$(C_5H_8)_n$
cis-Polypentenamer	$(C_5H_8)_n$
trans-Polypentenamer	$(C_5H_8)_n$
Polyphenylene PP-1	$C_{20.84}H_{16.66}O_{0.62}$
Polyphenylene PP-2	$C_{20.84}H_{16.66}O_{0.62}$
Poly-2,2'-*m*-phenylene)-5,5'-dibenzoxazole methane	$(C_{21}H_{12}N_2O_2)_n$
Poly-[2,2'-(*p*-phenylene-1,1-diphenyl-5,5'-dibenzimidazole]	$(C_{32}H_{20}N_4)_n$
Poly[2,2'-(1,4-phenylene)-7,7'-oxy-bis (3-phenylquinoxaline)]	$C_{34}H_{20}N_4O$
Polypropylene, isotatic, amorphous	$(C_3H_6)_n$
Polypropylene, isotatic, crystalline	$(C_3H_6)_n$
Poly-[N-terphthalyl-bis-(N'-phenyl-*o*-diphenylamine)]	$(C_{32}H_{24}N_4O_2)_n$
Polystyrene	$(C_8H_8)_n$
Polystyrene-d_3	$(C_8H_5D_3)_n$
Polystyrene-d_5	$(C_8H_3D_5)_n$
Polystyrene-d_8	$(C_8D_8)_n$
Polystyrene-Polystyrene-d_8	$(C_{16}H_8D_8)_n$
Polytetrahydrofuran	$(C_4H_8O)_n$
Polythene	$(CH_2)_n$
Polytriazine	$(C_{24}H_{12}N_6)_n$
Poly(tridecanolactone)	$(C_{13}H_{24}O_2)_n$
Poly-N-(β-trimethylsilylethyl)azetidine	$(C_8H_{19}NSi)_n$
Poly-N-(β-trimethylsilylethyl)ethylenimine	$(C_7H_{17}NSi)_n$
Polyvinyl alcohol	$(C_2H_4O)_n$
Polyvinyl chloride	$(C_2H_3Cl)_n$
Polyvinyldimethylbenzylsilane	$(C_{11}H_{16}Si)_n$
Polyvinyldimethylphenylsilane	$(C_{10}H_{14}Si)_n$
Polyvinylenediphenylsilyl,germyl-α,ω-dihydride copolymer	$(C_{28}H_{24}GeSi)_n$
Polyvinylenediphenylgermyl-α,ω-dihydride	$(C_{14}H_{12}Ge)_n$
Polyvinylenediphenylsilyl-α,ω-dihydride	$(C_{14}H_{12}Si)_n$
Polyvinylidene chloride	$(C_2H_2Cl_2)_n$
Polyvinyltrimethylsilane	$(C_5H_{12}Si)_n$
Potassium butyrate	$C_4H_7KO_2$
Potassium 2-methylpropanoate	$C_4H_7KO_2$
Potassium propionate	$C_3H_5KO_2$
Potassium tetraphenyl boron	$C_{24}H_{20}BK$
Propaldehyde	C_3H_6O
Propanal	C_3H_6O
n-Propane	C_3H_8
1,2-Propanediol	$C_3H_8O_2$
1,2,3-Propanetriol	$C_3H_8O_3$
Propanoic acid	$C_3H_6O_2$
1-Propanol	C_3H_8O
Propene	C_3H_6
β-Propiolactone	$C_3H_4O_2$
Propionic acid	$C_3H_6O_2$
4-Propionyl-4'-*n*-butanoyloxyazobenzene	$C_{19}H_{20}N_2O_3$
4-Propionyl-4'-*n*-decanoyloxyazobenzene	$C_{25}H_{32}N_2O_3$
4-Propionyl-4'-*n*-dodecanoyloxyazobenzene	$C_{27}H_{36}N_2O_3$
4-Propionyl-4'-*n*-heptadecanoyloxyazobenzene	$C_{32}H_{46}N_2O_3$
4-Propionyl-4'-*n*-heptanoyloxyazobenzene	$C_{22}H_{26}N_2O_3$
4-Propionyl-4'-*n*-hexadecanoyloxyazobenzene	$C_{31}H_{44}N_2O_3$
4-Propionyl-4'-*n*-hexanoyloxyazobenzene	$C_{21}H_{24}N_2O_3$
4-Propionyl-4'-*n*-nonanoyloxyazobenzene	$C_{24}H_{30}N_2O_3$
4-Propionyl-4'-*n*-octadecanoyloxyazobenzene	$C_{33}H_{48}N_2O_3$
4-Propionyl-4'-*n*-octanoyloxyazobenzene	$C_{23}H_{28}N_2O_3$
4-Propionyl-4'-*n*-pentadecanoyloxyazobenzene	$C_{30}H_{42}N_2O_3$
4-Propionyl-4'-*n*-tetradecanoyloxyazobenzene	$C_{29}H_{40}N_2O_3$
4-Propionyl-4'-*n*-tridecanoyloxyazobenzene	$C_{28}H_{38}N_2O_3$
4-Propionyl-4'-*n*-undecanoyloxyazobenzene	$C_{26}H_{34}N_2O_3$
n-Propyl acetate	$C_5H_{10}O_2$
n-Propyl alcohol	C_3H_8O
Propyl ethanoate	$C_5H_{10}O_2$
Propyl formate	$C_4H_8O_2$
Propyl methanoate	$C_4H_8O_2$
n-Propyl methyl ketone	$C_5H_{10}O$
n-Propyl propanoate	$C_6H_{12}O_2$
Propyl propionate	$C_6H_{12}O_2$
Propyl urea	$C_4H_{10}N_2O$
Propyldiammonium cadmium tetrachloride	$C_3H_{12}CdCl_4N_2$
Propyldiammonium manganese tetrachloride	$C_3H_{12}Cl_4MnN_2$
Propylene carbonate	$C_4H_6O_3$
Propylene glycol	$C_3H_8O_2$
Propylene oxide clathrate hydrate	$C_3H_6O{\cdot}17H_2O$
Propylene oxide	C_3H_6O
Propylene	C_3H_6
Pyrazole	$C_3H_4N_2$
Pyrene picric acid	$C_{22}H_{13}N_3O_7$
Pyrocatechin	$C_6H_6O_2$
Pyromellitic dianhydride	$C_{10}H_2O_6$
α-Pyrrolidone	C_4H_7NO
Pyrroyl manganese tricarbonyl	$C_7H_4MnNO_3$

Q

Quadricyclane	C_7H_8
p-Quaterphenyl	$C_{24}H_{18}$
Quinoline	C_9H_7N
p-Quinquephenyl	$C_{30}H_{22}$

R

Resorcin	$C_6H_6O_2$
Resorcinol	$C_6H_6O_2$
Ribose(D)	$C_5H_{10}O_5$
Rochelle salt	$C_4H_4KNaO_6{\cdot}4H_2O$
Rubidium tetraphenyl boron	$C_{24}H_{20}BRb$
Ruthenocene	$C_{10}H_{10}Ru$

S

β-Selenodiglycol	$C_4H_{10}O_2Se$
Selenophene chromium tricarbonyl	$C_7H_4CrO_3Se$
Semicarbazide	CH_5N_3O
Silver phenylacetylenide	C_8H_5Ag
Sodium acetate	$C_2H_3NaO_2$
Sodium acetate trihydrate	$C_2H_3NaO_2{\cdot}3H_2O$

Sodium ethanoate	$C_2H_3NaO_2$
Sodium formate	$CHNaO_2$
Sodium methanoate	$CHNaO_2$
Sodium potassium tartrate tetrahydrate	$C_4H_4KNaO_6{\cdot}4H_2O$
Sodium propanoate	$C_3H_5NaO_2$
Sorbitol(D)	$C_6H_{14}O_6$
Squaric acid	$C_4H_2O_4$
Stearic acid	$C_{18}H_{36}O_2$
trans-Stilbene	$C_{14}H_{12}$
Strontium dicalcium propionate	$C_{18}H_{30}Ca_2O_{12}Sr$
Styphnic acid	$C_6H_3N_3O_8$
Styrene	C_8H_8
Styrene-d_8	C_8D_8
Succinonitrile	$C_4H_4N_2$
Sucrose	$C_{12}H_{22}O_{11}$

T

Tellurophene chromium tricarbonyl	$C_7H_4CrO_3Te$
Terephthaloyl chloride	$C_8H_4Cl_2O_2$
p-Terphenyl	$C_{18}H_{14}$
Terephthalodinitrile	$C_8H_4N_2$
3,3',4,4'-Tetraaminodiphenyl ether	$C_{12}H_{12}N_4O$
1,4,8,11-Tetraazacyclotetradecane	$C_{10}H_{24}N_4$
Tetrabromomethane	CBr_4
1,2,4,5-Tetrachlorobenzene	$C_6H_2Cl_4$
Tetrachlorobis-(butylammonium) manganese II	$C_8H_{24}Cl_4MnN_2$
Tetrachlorobis-(decylammonium) manganese II	$C_{20}H_{48}Cl_4MnN_2$
Tetrachlorobis-(deuteromethylammonium) manganese II	$C_2H_6Cl_4D_6MnN_2$
Tetrachlorobis-(ethylammonium) manganese II	$C_4H_{16}Cl_4MnN_2$
Tetrachlorobis-(methylammonium) manganese II	$C_2H_{12}Cl_4MnN_2$
Tetrachlorobis-(pentylammonium) manganese II	$C_{10}H_{28}Cl_4MnN_2$
Tetrachlorobis-(propylammonium) manganese II	$C_6H_{20}Cl_4MnN_2$
1,1,1,2-Tetrachlorodifluoroethane	$C_2Cl_4F_2$
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$
Tetrachloroethane	C_2Cl_4
Tetrachloroethylene	C_2Cl_4
Tetrachloromethane	CCl_4
n-Tetracosane	$C_{24}H_{50}$
Tetracyclo[3.2.0.0.^{2,7}.0^{4,6}]heptane	C_7H_8
n-Tetradecane	$C_{14}H_{30}$
1-Tetradecanethiol	$C_{14}H_{30}S$
n-Tetradecyl mercaptan	$C_{14}H_{30}S$
Tetraethylammonium tetrabromoferrate	$C_8H_{20}Br_4FeN$
Tetraethylammonium tetrachloroferrate	$C_8H_{20}Cl_4FeN$
1,1,3,3-Tetraethyl-5,5-dimethylcyclotrisiloxane	$C_{10}H_{26}O_3Si_3$
1,1,3,3-Tetraethyl-5,5-diphenylcylotrisiloxane	$C_{16}H_{22}O_3Si_3$
Tetraethylene glycol	$C_8H_{18}O_5$
Tetraethylenepentamine	$C_8H_23N_5$
Tetraethylgermane	$C_8H_{20}Ge$
Tetraethylgermanium	$C_8H_{20}Ge$
Tetraethyllead	$C_8H_{20}Pb$
Tetraethylmethane	C_9H_{20}
Tetraethylsilicon	$C_8H_{20}Si$
Tetraethyltin	$C_8H_{20}Sn$
Tetrafluoromethane	CF_4
1,2,3,4-Tetrahydroanthracene	$C_{14}H_{14}$
Tetrahydrofuran	C_4H_8O
Tetrahydrofuran clathrate hydrate	$C_4H_8O{\cdot}17H_2O$
Tetrahydro-1,4-isoxazine	C_4H_9NO
exo-Tetrahydrodicyclopentadiene	$C_{10}H_{16}$
1,2,3,4-Tetrahydrophenanthrene	$C_{14}H_{14}$
1,2,3,4-Tetrahydroquinoline	$C_9H_{11}N$
5,6,7,8-Tetrahydroquinoline	$C_9H_{11}N$
Tetramethylammonium hexacyanotrimethylenecyclopropanide	$C_{16}H_{12}N_7$
Tetramethylammonium tetrachloroferrate	$C_8H_{24}Cl_4FeN_2$
Tetramethylammonium tetrachloroferrate (III)	$C_4H_{12}Cl_4FeN$
Tetramethylammonium tetrachloromanganate	$C_8H_{24}Cl_4MnN_2$
Tetramethylammonium trichloromanganate(II)	$C_4H_{12}Cl_3MnN$
1,1,3,3-Tetramethyl-1,3-disilacyclobutane	$C_6H_{16}Si_2$
2,4,5,7-Tetramethyl-4,5-bis(4-*tert*-butylphenyl)octane	$C_{32}H_{50}$
1,1,10,10-Tetramethylcyclooctadecane	$C_{22}H_{44}$
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane	$C_{16}H_{22}OSi_2$
Tetramethyl germane	$C_4H_{12}Ge$
3,7,11,15-Tetramethyl-1-hexadecyn-3-ol	$C_{20}H_{40}O$
3,7,11,15-Tetramethyl-1-hexadecen-3-ol	$C_{20}H_{40}O$
Tetramethylhex-3-ene	$C_{10}H_{20}$
Tetramethyl lead	$C_4H_{12}Pb$
2,2,4,4-Tetramethyl-3-oxapentane	$C_8H_{18}O$
2,2,3,3-Tetramethylpentane	C_9H_{20}
2,2,4,4-Tetramethylpentane	C_9H_{20}
N,N,N',N'-Tetramethyl-*p*-phenylenediamine perchlorate	$C_{10}H_{16}N_2ClO_4$
Tetra(methylphenyl)tetrasiloxane	$C_{28}H_{32}Si_4O_4$
Tetramethyl silicate	$C_4H_{12}O_4Si$
Tetramethyl stannane	$C_4H_{12}Sn$
Tetramethyl tin	$C_4H_{12}Sn$
Tetramethylurea	$C_5H_{14}N_2O$
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(α)	$C_4H_8N_8O_8$
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine(β)	$C_4H_8N_8O_8$
1,3,5,7-Tetranitro-1,3,5,7-tetrazocine	$C_4H_8N_8O_8$
Tetrapropylene glycol	$C_{12}H_{26}O_5$
n-Tetratriacontane	$C_{34}H_{70}$
Thallium acetate	$C_2H_3O_2Tl$
Thallium butyrate	$C_4H_7O_2Tl$
Thallium decanoate	$C_{10}H_{19}O_2Tl$
Thallium dodecanoate	$C_{12}H_{23}O_2Tl$
Thallium formate	CHO_2Tl
Thallium heptanoate	$C_7H_{13}O_2Tl$
Thallium hexadecanoate	$C_{16}H_{31}O_2Tl$
Thallium hexanoate	$C_6H_{11}O_2Tl$
Thallium nonanoate	$C_9H_{17}O_2Tl$
Thallium octadecanoate	$C_{18}H_{35}O_2Tl$
Thallium octanoate	$C_8H_{15}O_2Tl$
Thallium pentanoate	$C_5H_9O_2Tl$
Thallium propionate	$C_3H_5O_2Tl$
Thallium tetradecanoate	$C_{14}H_{27}O_2Tl$
Thioacetamide	C_2H_5NS
Thiobenzamide	C_7H_7NS
Thiocarbohydrazide	CH_6N_4S
Thiophene chromium tricarbonyl	$C_7H_4CrO_3S$
Thiophene	C_4H_4S
Thiosemicarbazide	CH_5N_3S
Thiourea	CH_4N_2S
Thiourea nitrate	$CH_4N_2S{\cdot}HNO_3$
Thymine	$C_5H_6N_2O_2$
α-Tocopherol	$C_{31}H_{52}O_3$

Toluene	C_7H_8
p-Toluidine	C_7H_9N
1,2,4-Triazole	$C_2H_3N_3$
Triacetin	$C_9H_{14}O_6$
n-Triacontane	$C_{30}H_{62}$
Triazine triol	$C_3H_3N_3O_3$
2,4,6-Tribromoaniline	$C_6H_3Br_3N$
Tribromomethane	$CHBr_3$
2,4,6-Tribromophenol	$C_6H_3Br_3O$
Tri-*tert*-butyl methanol	$C_{13}H_{28}O$
Tri-*n*-butylphosphate	$C_{12}H_{27}O_4P$
Tributyrin	$C_{15}H_{26}O_6$
Trichloroacetic acid	$C_2HCl_3O_2$
1,2,4-Trichlorobenzene	$C_6H_3Cl_3$
1,1,1-Trichloroethane	$C_2H_3Cl_3$
1,1,2-Trichloroethane	$C_3H_3Cl_3$
Trichloroethene	C_2HCl_3
Trichloroethylene	C_2HCl_3
Trichlorofluoroethene	C_2ClF_3
Trichlorofluoroethylene	C_2ClF_3
Trichloromethane	$CHCl_3$
Trichloromethylsilane	CH_3Cl_3Si
p-Trichlorosilylbiphenyl	$C_{12}H_9Cl_3Si$
β-Trichlorosilylpropionitrile	$C_3H_4Cl_3Si$
α,α,α-Trichlorotoluene	$C_7H_5Cl_3$
1,1,1-Trichlorotrifluoroethane	$C_2Cl_3F_3$
1,1,2-Trichlorotrifluoroethane	$C_2Cl_3F_3$
Tricosane	$C_{23}H_{48}$
n-Tricosane	$C_{23}H_{48}$
Tricresyl phosphate	$C_{21}H_{21}O_4P$
Tricyclopentadienyl yttrium	$C_{15}H_{15}Y$
Tricyclo[2.2.1.0^{2,6}]heptane	C_7H_{10}
Tricyclo[3.3.2.0^{4,6}]deca-2,7,9-triene	$C_{10}H_{10}$
Tridecanolactone	$C_{13}H_{24}O_2$
Triethanolamine	$C_6H_{15}NO_3$
Triethanolamine borate	$C_6H_{12}BNO_3$
Triethyl aluminum	$C_6H_{15}Al$
Triethyl arsine	$C_6H_{15}As$
Triethyl boron	$C_6H_{15}B$
Triethylene glycol	$C_6H_{14}O_4$
Triethylenetetramine	$C_6H_{18}N_4$
Triethyl gallium	$C_6H_{15}Ga$
Trifluoroacetyl fluoride	C_2F_4O
α-(Trifluoromethoxy)-α,α-difluoromethyl acetate	$C_4H_3F_5O_3$
3-Trifluoromethylbenzoic acid	$C_7H_5F_3O_2$
Trifluoromethyl (2-hydroxy-1-propenyl) ketone	$C_5H_5F_3O_2$
3-Trifluoromethyl nitrobenzene	$C_7H_4F_3NO_2$
m-Trifluorotoluic acid	$C_7H_5F_3O_2$
Triglycine fluoroberyllate-d_x	$C_6D_{17}BeF_4N_3O_6$
Triglycine fluoroberyllate, deuterated	$C_6D_{17}BeF_4N_3O_6$
Triglycine fluoroberyllate	$C_6H_{17}BeF_4N_3O_6$
Triglycine sulfate, deuterated	$C_6D_{17}N_3O_{10}S$
Triglycine sulfate-triglycine selenate	$C_6H_{17}N_3O_{10}S{\cdot}C_6H_{17}N_3O_{10}Se$
Triglycine sulfate	$C_6H_{17}N_3O_{10}S$
1,1,1-Trihydroxymethyl propane	$C_4H_{10}O_3$
1,2,3-Trihydroxypropane	$C_3H_8O_3$
Trimargarin	$C_{54}H_{104}O_6$
Trimethylaluminum	C_3H_9Al
Trimethyl arsine	C_3H_9As
2,5,6-Trimethyl-2-cyclohexen-1-one	$C_9H_{14}O$
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	$C_{13}H_{20}O$
3,7,11-Trimethyl-1-dodecen-3-ol	$C_{15}H_{28}O$
Trimethyl gallium	C_3H_9Ga
Trimethylhydroquinone	$C_9H_{12}O_2$
6,10,14-Trimethyl-2-pentadecanone	$C_{18}H_{36}O$
6,10,14-Trimethyl-3,5-pentadecadien-2-one	$C_{18}H_{32}O$
2,2,4-Trimethylpentane	C_8H_{18}
2,5,6-Trimethylphenol	$C_9H_{12}O$
cis-Tri(methylphenyl)trisiloxane	$C_{21}H_{24}Si_3O_3$
trans-Tri(methylphenyl)trisiloxane	$C_{21}H_{24}Si_3O_3$
N-(β-Trimethylsilylethyl) ethylenimine	$C_7H_{17}NSi$
N-(β-Trimethylsilylethyl)azetidine	$C_8H_{19}NSi$
1,3,6-Trimethyluracil	$C_7H_{10}N_2O_2$
1,1,3-Trimethylurea	$C_4H_{10}N_2O$
2,4,6-Trinitrophenol	$C_6H_3N_3O_7$
2,4,6-Trinitroresorcinol	$C_6H_3N_3O_8$
1,3,5-Trioxane	$C_3H_6O_3$
2,5,8-Trioxanonane	$C_6H_{14}O_3$
1,3,5-Triphenylbenzene	$C_{24}H_{18}$
Triphenylchlorosilane	$C_{18}H_{15}ClSi$
Triphenylene picric acid	$C_{24}H_{15}N_3O_7$
Triphenyl phenylethynyl tin	$C_{26}H_{20}Sn$
Triphenyl phosphate	$C_{18}H_{15}O_4P$
Triphenylphosphine	$C_{18}H_{15}P$
Triphenylphosphine oxide	$C_{18}H_{15}OP$
2,4,6-Triphenylpyridine	$C_{23}H_{17}N$
Triphenyl-s-triazine	$C_{21}H_{15}N_3$
Triphenyl vinyl tin	$C_{20}H_{18}Sn$
Tripropionin	$C_{12}H_{20}O_6$
Tripropylaluminum	$C_9H_{21}Al$
Tripropylene glycol	$C_9H_{20}O_4$
Triptycene	$C_{20}H_{14}$
Trisarcosine calcium chloride	$C_9H_{21}N_3O_6CaCl_2$
Tris-(cyclopentadienylcobalt) disulfide	$C_{15}H_{15}Co_3S_2$
Tris(2-picolylamine)iron chloride ethanolate	$C_{20}H_{33}Cl_2FeN_6O$
Tristearin	$C_{57}H_{110}O_6$
anti,trans-Truxane	$C_{18}H_{16}$
syn,trans-Truxane	$C_{18}H_{16}$

U

6-Undecanone	$C_{11}H_{22}O$
Undecylcyanobiphenyl	$C_{24}H_{31}N$
Urea	CH_4N_2O
Urethane	$C_3H_7NO_2$

V

Valeral	$C_5H_{10}O$
Valeraldehyde	$C_5H_{10}O$
δ-Valerolactone	$C_5H_8O_2$
Valeronitrile	C_5H_9N
Vanadocene	$C_{10}H_{10}V$
Vinyl chloride	C_2H_3Cl
Vinyldimethylbenzylsilane	$C_{11}H_{16}Si$
Vinyldimethylphenylsilane	$C_{10}H_{14}Si$
Vinyltrimethylsilane	$C_5H_{12}Si$

W

Wurster's Blue perchlorate	$C_{10}H_{16}N_2ClO_4$

X

p-Xylene	C_8H_{10}
Xylose(D)	$C_5H_{10}O_5$

Z

Zinc acetate	$C_4H_6O_4Zn$
Zinc acetate dihydrate	$C_4H_6O_4Zn{\cdot}2H_2O$
Zinc acetylacetonate	$C_{10}H_{14}ZnO_4$
Zirconium acetylacetonate	$C_{20}H_{28}ZrO_6$

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89RAB/NIS2 Rabinovich, I. B., Nistratov, V. P., Sheiman, M. S., Karataev, E. N., Kamelova, G. P., and Feshchenko, I. A., Heat capacity, phase transitions, and thermodynamic functions of tetraethyllead, Zhur. Fiz. Khim. **63**, 2520–2524 (1989).

89SHE/RAB Sheiman, M. S., Rabinovich, I. B., Nistratov, V. P., Kamelova, G. P., Karataev, E. N., and Feshchenko, I. A., Specific heat and thermodynamic characteristics of tetramethylstanane, Zhur. Fiz. Khim. **63**, 836–838 (1989).

89STE/CHI Steele, W. V., Chirico, R. D., Hossenlopp, I. A., Nguyen, A., Smith, N. K., and Gammon, B. E., The thermodynamic properties of five benzoquinolines, J. Chem. Thermodynam. **21**, 81–107 (1989).

89STE/CHI2 Steele, W. V., Chirico, R. D., Hossenlopp, I. A., Nguyen, A., Smith, N. K., and Gammon, B. E., The thermodynamic properties of 1,2,3,4- and 5,6,7,8-tetrahydroquinoline, J. Chem. Thermodynam. **21**, 1121–1149 (1989).

89VES/BAR Vesely, F., Barcal, P., Zabransky, M., and Svoboda, V., Heat capacities of 4-methyl-2-pentanone, 2,6-dimethyl-4-heptanone, 1-hexanol, 1-heptanol, and 1-octanol in the temperature range 298–318 K, Collect. Czech. Chem. Commun. **54**, 602–607 (1989).

89YOS/SOR Yoshikawa, M., Sorai, M., and Suga, H., Heat capacity of a five-coordinated iron (III) complex with spin 3/2, bromobis(N,N-dimethylcarbamato) iron (III), between 0.4 and 300 K: new finding of a magnetic phase transition, J. Phys. Chem. Solids **50**, 713–722 (1989).

89ZHA/YAN Zhang, Z. Y., and Yang, M. L., Heat capacities and phase transitions of 1,1,1-trihydroxymethylpropane and pentaerythritol over the superambient temperature range, Thermochim. Acta **156**, 157–161 (1989).

10. Appendix: Errata for "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase"

[J. Phys. & Chem. Ref. Data 13, Suppl. No.1, 286 pp. (1984)]

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The errata are arranged in the format shown below and are listed as found according to successive pages in the 1984 publication, J. Phys. Chem. Ref. Data **13**, Suppl. 1 (1984). After the page number for a specific erratum, which is shown on the extreme left side of the first line, information is provided regarding its location on a given page, such as: compound formula, compound name, reference squib, or other pertinent information. On the second line, the erratum appears as found in the publication. On the third line, one finds the correction. The last line offers a comment or explanation about the erratum.

Errata Format
Page Formula/Name/Reference/Text Incorrect (as it appears) Correct (as it should be) [comment regarding error]

Specific Errata

6 **5. Definitions**, 3rd paragraph, lines 3 and 4
Incorrect ...and is referred to the midpoint of ...
$...C_p = \Delta H/(T_2 - T_1), (T_2 - T_1)/2.$
Correct ...and is referred to *as* the midpoint of ...
$...C_p = \Delta H/(T_2 - T_1), (T_1 + T_2)/2.$
[missing word and formula error]

10 C Graphite 80TAY/GRO
Incorrect Wiswesser Line Notation ...
Correct Wiswesser Line Notation C
[WLN absent]

11 CCl_3F Fluorotrichloromethane 40BEN/MCH
Incorrect Wiswesser Line Notation GYGGF
Correct Wiswesser Line Notation GXGGF
[WLN error]

14 $CHCl_2F$ Dichlorofluoromethane 40BEN/MCH
$C_p = 112.6$ J·mol^{-1}·K^{-1}
[C_p value in J·mol^{-1}·K^{-1} repeated]

24 $C_2Br_2F_4$ 1,2-Dibromotetrafluoroethane 82KOS/ZHO
Incorrect WLN FXFFEXFFE
Correct WLN FXFEXFFE
[WLN error]

32 $(C_2H_3NO)_n$ Polyglycine I 81FIN/KUM
Incorrect molecular weight 75.0670
Correct molecular weight 57.0518
[numerical error]

32 $(C_2H_3NO)_n$ Polyglycine II 81FIN/KUM
Incorrect molecular weight 75.0670
Correct molecular weight 57.0518
[numerical error]

33 $C_2H_4Br_2$ 1,2-Dibromoethane 40PIT 2
Incorrect Phase Changes...c/I/liq...
Correct Phase Changes...c,I/liq...
[typographical error]

42 $C_2H_{12}CdCl_4N_2$ Tetrachlorobis-(methylammonium) cadmium II 81RAH/CLA
Incorrect WLN CD ZI&2 G4
Correct WLN ZH&1 2 -CD- G4
[WLN error]

42 $C_2H_{12}Cl_4MnN_2$ Tetrachloro-(methylammonium) manganese II 82WHI/GRA
Incorrect WLN MN Z1&2 G4
Correct WLN ZH&1 2 -MN- G4
[WLN error]

43 $C_{2.2}H_{6.5}N_2O$ Urea-1-dodecene adduct 72GAN/PAR
Incorrect WLN 11U1 &ZVZ
Incorrect molecular weight 77.8975
Correct WLN ZVZ &11U1 0.1060
Correct molecular weight 76.9884
Mole ratio of 1-dodecene to urea = 0.1060
[WLN and molecular weight error]

43 $C_{2.2}H_{6.6}N_2O$ Urea-*n*-undecane adduct 69COP/PAR
Incorrect WLN ZVZ &11H
Incorrect molecular weight 77.2496
Correct WLN ZVZ &11H 0.1104
Correct molecular weight 77.0892
Mole ratio of *n*-undecane to urea = 0.1104
[WLN and molecular weight error]

43 $C_{2.3}H_{6.7}N_2O$ Urea-1-hexadecene adduct 69COP/PAR
Incorrect WLN 15U1 &ZVZ
Incorrect molecular weight 79.3563
Correct WLN ZVZ &15U1 0.0860
Correct molecular weight 78.3911
Mole ratio of 1-hexadecene to urea = 0.0860
[WLN and molecular weight error]

44 $C_{2.3}H_{6.7}N_2O$ Urea-1-decene adduct 69COP/PAR
Incorrect WLN ZVZ &9U1
Incorrect molecular weight 79.2721
Correct WLN ZVZ &9U1 0.1370
Correct molecular weight 78.3911
Mole ratio of 1-decene to urea = 0.1370
[WLN and molecular weight error]

44 $C_{2.4}H_{6.8}N_2O$ Urea-1-octadecene adduct 72GAN/PAR
Incorrect WLN 17U1 &ZVZ
Incorrect molecular weight 79.8893
Correct WLN ZVZ &17U1 0.0785
Correct molecular weight 79.6930
Mole ratio of 1-octadecene to urea = 0.0785
[WLN and molecular weight error]

44 $C_{2.4}H_{6.8}N_2O$ Urea-1-eicosene adduct 69COP/PAR
Incorrect WLN 19U1 &ZVZ
Incorrect molecular weight 79.6929
Correct WLN ZVZ &19U1 0.0704
Correct molecular weight 79.6930
Mole ratio of 1-eicosene to urea = 0.0704
[WLN and molecular weight error]

44 **$C_{2.4}H_{6.9}N_2O$** (c) 72GAN/PAR
Urea-1-tetradecene adduct; 1-Tetradecene-urea adduct
Heat Capacity 298.15 K $C_p = 30.9$ cal·mol^{-1}·K^{-1}
129.2 J·mol^{-1}·K^{-1}
Temperature range 12–300 K. Values for one mole urea in adduct.
Entropy 298.15 K, $S = 34.7$ cal·mol^{-1}·K^{-1}
145.1 J·mol−1·K^{-1}
Does not include possible zero-point entropy.
Phase Changes
Anomalous region 225–235 K,
with $\Delta H = 15$ J·mol^{-1} (urea) and $\Delta S = 0.067$ J·mol^{-1}·K^{-1}.
c,II/c,I 256.6 K $\Delta H = 868.5$ cal·mol^{-1}
3634 J·mol^{-1}
$\Delta S = 2.9$ cal·mol^{-1}·K^{-1}
12.0 J·mol^{-1}·K^{-1}
Molecular Weight 80.0660
Wiswesser Line Notation ZVZ &13U1 0.1019
Evaluation B
[Data in 72GAN/PAR omitted from tables]

45 $C_3H_2N_2$ Malononitrile 68WES/WUL
Incorrect Reference 68WES/WUL
Correct Reference 68GIR/WES
[Incorrect reference citation; see also erratum for page 278]

52 C_3H_6O 3-Propenol; Allyl alcohol 81REI
Incorrect 3-Propen-1-ol
Incorrect WLN Q1U2
Correct 2-Propen-1-ol
Correct WLN Q2U1

[nomenclature and WLN error]

54 C_3H_7NO N,N-Dimethylmethanamide 66GEL
Incorrect 66GEL
Correct 61GEL
[reference error; see also erratum on page 277]

55 $C_3H_7NO_2$ 2-Aminopropanoic acid (L) 75DAU/DEL
Incorrect WLN ZYVQ -L
Correct WLN ZY1&VQ -L
[WLN error]

66 $C_4H_6KNaO_6.4H_2O$ Sodium potassium tartrate tetrahydrate 78TAT/MAT
Incorrect $C_4H_6KNaO_6{\cdot}4H_2O$
Incorrect Molecular Weight 284.2367
Correct $C_4H_4KNaO_6{\cdot}4H_2O$
Correct Molecular Weight 282.2209
[formula and molecular weight error]

68 $C_4H_7NO_4$ Aminosuccinic acid (L); Aspartic acid (L) 63HUT/COL 2
Incorrect WLN ZVYZ1VQ -L
Correct WLN QVYZ1VQ -L
[typographical error]

71 C_4H_8O Butanal; n-Butryaldehyde 56PAR/KEN
Incorrect n-Butryaldehyde
Correct *n*-Butyraldehyde
[spelling error]

76 C_4H_{10} Butane 40AST/MES
Incorrect $C_p = 13242$ J·mol^{-1}·K^{-1}
Correct $C_p = 132.42$ J·mol^{-1}·K^{-1}
[decimal point omitted]

83 $C_4H_{12}Pb$ Tetramethyllead 59GOO/SCO
Incorrect phase (c)
Correct phase (liq)
[$T_m = 242.9$ K, hence, at 298.15 K, data for C_p and S for $C_4H_{12}Pb$ are for the liquid]
Incorrect entropy temperature 298.16 K
Correct entropy temperature 298.15 K
[transcription errors]

87 $C_5H_7N_2O_2$ Thymine 73ALV/BIL
Incorrect formula $C_5H_7N_2O_2$
Incorrect molecular weight 127.1225
Correct formula $C_5H_6N_2O_2$
Correct molecular weight 126.1146
[formula and molecular weight error]

87 $CH_7N_2O_2$ Thymine 78KIL2
Incorrect formula $C_5H_7N_2O_2$
Incorrect molecular weight 127.1225
Correct formula $C_5H_6N_2O_2$
Correct molecular weight 126.1146
[formula and molecular weight error]

91 $C_5H_8O_2$ Ethenyl ethanoate; Allyl acetate 81REI
Incorrect Ethenyl ethanoate
Correct 2-Propenyl ethanoate
[nomenclature error]

91 $(C_5H_8O_2)_n$ Polymethylmethacrylate 58SOC/TRA
Incorrect WLN /*X1&*VO1/
Correct WLN /*X1*1&VO1/
[WLN error]

93 C_5H_{10} 1-Pentene 30PAR/HUF 2
Incorrect 1-Pentene
Incorrect WLN 4U1
Correct 2-Pentene
Correct WLN 3U2
[30PAR/HUF 2 measured 2-Pentene, liquid]

101 $C_5H_{12}O$ 2,2-Dimethyl-1-propanol; tert-Amyl alcohol 33PAR/HUF
Incorrect 2,2-Dimethyl-1-propanol; tert-Amyl alcohol
Incorrect WLN Q1X1&1&1
Correct 2-Methyl-2-butanol; *tert*-Amyl alcohol
Correct WLN QX1&1&2
[nomenclature and WLN errors]

103 $C_5H_{12}S$ 2-Methyl-2-butanethiol; tert-Amyl mercaptan 74MES/FIN
Incorrect 2-Methyl-2-butanethiol; tert-Amyl mercaptan.....
Correct 3-Methyl-2-butanethiol
[nomenclature error; 74MES/FIN measured six mercaptans among which were both 3-methyl-1-butanethiol and 3-methyl-2-butanethiol]

104 $C_5H_{14}N_2$ 82DZH/KAR2
N,N-Dimethyl-1,3-propanediamine
Incorrect Molecular weight 130.1924
Incorrect WLN Z3NI&1
Correct Molecular weight 102.1790
Correct WLN Z3N1&1
[Molecular weight and WLN errors]

108 $C_6H_3N_3O_6$ 1,3,5-Trinitrobenzene 80RAD/RAD
Incorrect Molecular weight 181.4487
Correct Molecular weight 213.1064
[Molecular weight error]

108 $C_6H_3N_3O_7$ 2,4,6-Trinitrophenol; Picric acid 24TAY/RIN
Incorrect C_p = 57.3 cal·mol^{-1}K^{-1}
223.9 J·mol^{-1}·K^{-1}
Correct C_p = 57.3 cal·mol^{-1}·K^{-1}
239.7 J·mol^{-1}·K^{-1}
[numerical error]

110 $C_6H_4O_3$ Phthalic anhydride 36PAR/TOD
Incorrect $C_6H_4O_3$
Incorrect Molecular Weight 124.0958
Correct $C_8H_4O_3$
Correct Molecular Weight 148.1178

110 C_6H_5Br Bromobenzene 81REI
Incorrect WLN BR
Correct WLN ER
[WLN error]

116 $C_6H_6N_2O_2$ 3-Nitroaniline 26AND/LYN
Incorrect (c/liq) temperature 285.0 K
Correct (c/liq) temperature 385.0 K
[temperature error]

129 $C_6H_{12}S$ Cyclohexanethiol; Cyclohexyl mercaptan 67MES/TOD
Incorrect C_p = 6.04 cal·mol^{-1}·K^{-1}
Correct C_p = 46.04 cal·mol^{-1} ·K^{-1}
[numerical error]

130 $C_6H_{13}N_3O_8S$ Triglycine sulfate 68AGU/TEL
Incorrect formula $C_6H_{13}N_3O_8S$
Incorrect Mol. Wt. 287.2440
Incorrect WLN Z1VM1VM1VQ &WSQQ
Correct formula $C_6H_{17}N_3O_{10}S$
Correct Mol. Wt. 323.2804
Correct WLN Z1VQ 3 &WSQQ
[error in formula, molecular weight, and WLN]

131 $C_6H_{13}N_3O_8S$ Triglycine sulfate 80RAM/CER
Incorrect C_p = 90.6 cal·mol^{-1}·K^{-1}
379.1 J·mol^{-1}·K^{-1}
Incorrect formula $C_6H_{13}N_3O_8S$
Incorrect Mol. Wt. 287.2440
Incorrect WLN Z1VM1VM1VQ &WSQQ
Correct C_p = 102.0 cal·mol^{-1}K^{-1}
426.7 J·mol^{-1}K^{-1}
Correct formula $C_6H_{17}N_3O_{10}S$
Correct Mol. Wt. 323.2804
Correct WLN Z1VQ 3 &WSQQ
[error in C_p, formula, molecular weight, and WLN]

136 $C_6H_{15}In$ Triethylindium 73MAS/NOV
[Data entry appears twice]

136 $C_6H_{16}CdCl_4N_2$ Tetrachlorobis-(2-propeneammonium) cadmium II 82WHI/STA
Incorrect WLN CD Z2U1&2 G4
Correct WLN Z2U1 2 -CD- G4
[WLN error]

137 $C_6H_{20}CdCl_4N_2$ Tetrachlorobis-(*n*-propylammonium) cadmium II 81WHI/GRA
Incorrect WLN CD Z3&2 G4
Correct WLN Z3H 2 -CD- G4
[WLN error]

137 $C_6H_{20}Cl_4MnN_2$ Tetrachlorobis-(*n*-propylammonium) manganese II 81WHI/GRA
Incorrect WLN MN Z3&2 G4
Correct WLN Z3H 2 -MN- G4
[WLN error]

141 $C_7H_6O_2$ Benzoic acid 53GIN/FUR
Incorrect temperature range 14-570 K
Correct temperature range 14-410 K
[numerical error]

157 C_8F_{16} Perfluorodimethylcyclohexane 57YAR/KAY
Incorrect WLN L6TJ AXFFF AF BF CF DF EF FF XXFFF XF
Correct WLN L6TJ AXFFF AF BF CF DF EF FF XXFFF XF XF XF XF
[WLN error]

158 C_8H_8 Styrene 50KUR
Incorrect C_p = 23.56 J·mol^{-1}·K^{-1}
Correct C_p =235.6 J·mol^{-1}·K^{-1}
[numerical error]

165 C_8H_{12} Cycloocta-1,5-diene 75LEB/TSV
[75LEB/TSV absent from bibliography; see erratum for page 282]

173 $C_8H_{18}O$ 2-Methyl-1-heptanol 31CLI/AND
Incorrect WLN QY5&1
Correct WLN Q1Y5&1
[WLN error]

179 $C_9H_{14}O_2$ Glyceryl triacetate 79FUC
Incorrect $C_9H_{14}O_2$
Incorrect Molecular Weight 154.2084
Correct $C_9H_{14}O_6$
Correct Molecular Weight 218.2060
[formula and molecular weight error]

191 $C_{10}H_{20}$ Diethylcyclohexane 63GUD/CAM
Incorrect C_p = 62.2 cal·mol^{-1}·K^{-1}
Incorrect temperature range 313-424 K
Correct C_p = 62.6 cal·mol^{-1}·K^{-1}
Correct temperature range 313-423 K
[numerical errors]

197 $C_{11}H_{26}N_2O$ Urea-*n*-decane adduct 65PEM/PAR
Incorrect spelling Value of aduct with...
Incorrect formula $C_{11}H_{26}N_2O$
Incorrect molecular weight 202.3392
Incorrect WLN ZVZ &10H
Correct spelling Value of adduct with...
Correct formula $C_{2.1}H_{6.5}N_2O$
Correct molecular weight 75.7876
Correct WLN ZVZ 10H 0.1149
Mole ratio of *n*-decane to urea = 0.1149
[spelling, formula, molecular weight, and WLN errors]

199 $C_{12}H_9N$ (c) Carbazole 80RAD/RAD
Heat Capacity 298.15 K C_p = 45.6 cal·mol^{-1}·K^{-1}
190.8 J·mol^{-1}·K^{-1}
Temperature range 180-410 *K*
$C_p = 54.87 + 0.2328T + 7.477 \times 10^{-4}T^2$
Phase Changes
c/liq 521.1 K ΔH = 6501 cal·mol^{-1}·K^{-1}
27200 J·mol^{-1}·K^{-1}
Molecular Weight 167.2098
Wiswesser Line Notation T B656 HMJ
Evaluation B
[Carbazole is in the name-formula index and bibliography, but not in the table of data for C_p, S, and phase changes. Data for carbazole should appear after data for $C_{12}H_9Cl_3Si$, *p*-Trichlorosilylbiphenyl]

203 $C_{12}H_{20}$ Tetracyclo[6.2.1.1^{3,6}]dodecane 62GOL/BEL
Incorrect Tetracyclo[6.2.1.1^{3,6}]dodecane
Incorrect WLN L D595 A D-TJ
Correct Tricyclo[6.2.1.1^{3,6}]dodecane
Correct WLN L59 D5 A D-TJ
[nomenclature error, also in 62GOL/BEL]

204 $C_{12}H_{22}O_2$ Dimethoxydecalin 63GUD/CAM
Incorrect $C_{12}H_{22}O_2$ Dimethoxydecalin
Incorrect Molecular Weight 198.3046
Incorrect WLN L66TJ XO1 XO1
Correct $C_{12}H_{18}$ Dimethanodecalin
Correct Molecular Weight 162.2742
Correct WLN L D5 C555 A D-TJ
[errors in formula, name, molecular weight, and WLN]

209 $C_{13}H_{30}N_2O$ Urea-*n*-dodecane adduct 65PEM/PAR
Incorrect spelling Value of aduct with...
Incorrect formula $C_{13}H_{30}N_2O$
Incorrect molecular weight 230.3928
Incorrect WLN ZVZ &12H
Correct spelling Value of adduct with...
Correct formula $C_{2.2}H_{6.3}N_2O$
Correct mol. wt. 76.7871
Correct WLN ZVZ &12H 0.09714
Mole ratio of *n*-dodecane to urea = 0.09714
[spelling, formula, molecular weight, and WLN errors]

209 $C_{13}H_{30}N_2O$ Urea-*n*-dodecane adduct 65PEM/PAR
Incorrect spelling Value of aduct with...
Incorrect formula $C_{13}H_{30}N_2O$
Incorrect mol. wt. 230.3928
Incorrect WLN ZVZ &12H
Correct spelling Value of adduct with
Correct formula $C_{2.2}H_{6.3}N_2O$
Correct mol. wt. 76.7871
Correct WLN ZVZ &12H 0.09714
Mole ratio of *n*-dodecane to urea = 0.09714
[spelling, formula, molecular weight, and WLN errors]

211 $C_{14}H_{10}O_2$ Benzil; Diphenyl diketone 77DWO/FUC
Incorrect .....data given graphicallyonly.
Correct .....data given graphically only.
[space missing]

224 $C_{17}H_{38}N_2O$ Urea-*n*-hexadecane adduct 65PEM/PAR
Incorrect formula $C_{17}H_{38}N_2O$
Incorrect mol. wt. 286.5000
Incorrect WLN ZVZ &16H
Correct formula $C_{2.3}H_{6.7}N_2O$
Correct mol. wt. 78.3914
Correct WLN ZVZ &16H 0.08057
Mole ratio on *n*-hexadecane to urea = 0.08057
[formula, molecular weight, and WLN errors]

224 $C_{18}H_{12}$ Naphthacene 80WON/WES
[80WON/WES not in bibliography; see erratum for page 285]

229-230 $C_{19}H_{21}ClNO$ *p*-*n*-Hexyloxybenzylideneamino-*p'*-chlorobenzene 77TSU/SOR
Incorrect WLN GR DNU1UR DO6
Correct WLN GR DNUYR DO6
[WLN error]

231 $C_{20}H_{12}$ Perylene 80WON/WES
[80WON/WES not in bibliography; see erratum for page 285]

232 $C_{20}H_{40}Br_2N_2$ 1,2-Bis(triallylammonium)ethane bromide 74BUR/VER
[data entry out of place; should follow data entry for $C_{20}H_{38}HgO_4$ Mercuric decanoate 78ADE]

234 $C_{21}H_{46}N_2O$ Urea-*n*-eicosane adduct 65PEM/PAR
Incorrect spelling Value for aduct with...
Incorrect formula $C_{21}H_{46}N_2O$
Incorrect mol. wt. 342.6072
Incorrect WLN ZVZ 20H
Correct spelling Value for adduct with...
Correct formula $C_{2.3}H_{6.8}N_2O$
Correct mol. wt. 78.4922
Correct WLN ZVZ &20H 0.06712
Mole ratio of *n*-eicosane to urea = 0.06712
[spelling, formula, molecular weight, and WLN errors]

236 $C_{24}H_{12}$ Coronene 80WON/WES
[80WON/WES not in bibliography; see erratum for page 285]

245 $C_{38}H_{72}O_4$ Di-*n*-tetradecyl sebacate 76PHI/MAT
Incorrect $C_{38}H_{72}O_4$
Incorrect Molecular Weight 592.9844
Correct $C_{38}H_{74}O_4$
Correct Molecular Weight 595.0002
[formula and molecular weight error]

245 $C_{41}H_{72}O_2$ Cholestryl myristate 67BAR/POR
Incorrect ...temperature range 270-270 K
Correct ...temperature range 270-370 K
[numerical error]

246 $C_{43}H_{26}N_8P$ Methyltriphenylphosphonium-bis(7,7,8,8-tetracyanoquinodomethanide) 77KOS/SOR 2
Incorrect Methyldiphenylphosphonium-bis(7,7,8,8-tetracyanoquinodomethanide)
Correct Methyldiphenylphosphonium-bis(7,7,8,8-tetracyanoquinodimethanide)
[nomenclature error]

250 **8. Compound Name - Formula Index**
Incorrect n-Butryaldehyde...
Correct *n*-Butyraldehyde...
[spelling error]

253 **8. Compound Name - Formula Index**
Incorrect Dimethoxydecalin ..... $C_{12}H_{22}O_2$
Correct Dimethanodecalin ..... $C_{12}H_{18}$
[error in name and formula]

253 **8. Compound Name - Formula Index**
Incorrect 2,2-Dimethyl-1-propanol ..... $C_5H_{12}O$
Correct .....
[delete entry]

254 **8. Compound Name - Formula Index**
Incorrect Ethenyl ethanoate ..... $C_5H_8O_2$
Correct 2-Propenyl ethanoate ..... $C_5H_8O_2$
[nomenclature error, relocate corrected name alphabetically]

254 **8. Compound Name - Formula Index**
Incorrect Freon 12 ..... $CHClF_2$
Correct Freon 12 ..... CCl_2F_2
[formula error]

255 **8. Compound Name - Formula Index**
Incorrect Glyceryl triacetate ..... $C_9H_{14}O_2$
Correct Glyceryl triacetate ..... $C_9H_{14}O_6$
[formula error]

257 **8. Compound Name - Formula Index**
Incorrect .....
Correct 2-Methyl-2-butanethiol ..... $C_5H_{12}S$
[name and formula omitted]

257 **8. Compound Name - Formula Index**
Incorrect 3-Metgylcyclohexanone
Correct 3-Methylcyclohexanone
[nomenclature error]

258 **8. Compound Name - Formula Index**
Incorrect Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodomethanide...
Correct Methyltriphenylphosphonium bis(7,7,8,8-tetracyanoquinodimethanide)...
[nomenclature error]

259 **8. Compound Name - Formula Index**
Incorrect Phthalic anhydride ..... $C_6H_4O_3$
Correct Phthalic anhydride ..... $C_8H_4O_3$
[formula error]

260 **8. Compound Name - Formula Index**
Incorrect 3-Propen-1-ol
Correct 2-Propen-1-ol
[numerical error]

260 **8. Compound Name - Formula Index**
Incorrect Sodium potassium tartrate tetrahydrate... ...$C_4H_6KNaO_6.4H_2O$
Correct Sodium potassium tartrate tetrahydrate... ...$C_4H_4KNaO_6.4H_2O$
[numerical error]

261 **8. Compound Name - Formula Index**
Incorrect Tetracyclo[6,2,1,$1^{3,6}$]dodecane...
Correct Tricyclo[6.2.1.$1^{3,6}$]dodecane...
[nomenclature error, relocate corrected name alphabetically]

262 **8. Compound Name - Formula Index**
Incorrect $C_6H_{13}N_3O_8S$ Triglycine sulfate
Correct $C_6H_{17}N_3O_{10}S$ Triglycine sulfate
[formula error]

262 **9. Compound Name - Formula Index**
Incorrect formula Urea-*n*-decane adduct $C_{11}H_{26}N_2O$
Incorrect formula Urea-*n*-dodecane adduct $C_{13}H_{30}N_2O$
Incorrect formula Urea-*n*-eicosnae adduct $C_{21}H_{46}N_2O$
Incorrect formula Urea-*n*-hexadecane adduct $C_7H_{38}N_2O$
Correct formula Urea-*n*-decane adduct $C_{2.1}H_{6.5}N_2O$
Correct formula Urea-*n*-dodecane adduct $C_{2.2}H_{6.3}N_2O$
Correct formula Urea-*n*-eicosane adduct $C_{2.3}H_{6.8}N_2O$
Correct formula Urea-*n*-hexadecane adduct $C_{2.3}H_{6.7}N_2O$
[formula error]

262 **8. Compound Name - Formula Index**
Incorrect name .....
Correct name Urea-1-tetradecene adduct $C_{2.4}H_{6.9}N_2O$
[compound name omitted from index]

265 **9. Bibliography**
Incorrect 31BLA/LET
Correct 31BLA/LEI
[tyopgrphical error]

265 **9. Bibliography**
Incorrect 31FIO/GIN ...881-800 (1931).
Correct 31FIO/GIN ...881-900 (1931).
[typographical error]

267 **9. Bibliography**
Incorrect 40AST/MES ...1917-1933 (1940).
Correct 40AST/MES ...1917-1923 (1940).
[numerical error]

267 **9. Bibliography**
Incorrect 40MES/AST
...J. Am. Chem. Soc. **62**, 887-890 (1940).
Correct 40MES/AST
...J. Am. Chem. Soc. **62**, 886-890 (1940).
[numerical error]

270 **9. Bibliography**
Incorrect 51SUG
...Bull. Chem. Soc. Japan **34**, 426-433 (1961).
Correct 61SUG
...Bull. Chem. Soc. Japan **34**, 426-433 (1961).
[numerical error]

271 **9. Bibliography**
Incorrect 52SCO/FIN
...functions, **74**, 2478-2483 (1952).
Correct 52SCO/FIN
...functions, J. Am. Chem. Soc. **74**, 2478-2483 (1952).
[journal citation absent]

271 **9. Bibliography**
Incorrect 53RAT/GWI ...5629 (1953).
Correct 53RAT/GWI ...5629-5633 (1953).
[numerical error]

271 **9. Bibliography**
Incorrect 54MCC/FIN 2 ...J. Am. Chem. Soc. **78**,...
Correct 54MCC/FIN 2 ...J. Am. Chem. Soc. **76**,...
[numerical error]

272 **9. Bibliography**
Incorrect 56FIN/SCO...1,3,5-cyclo-oD heptatriene...
Correct 56FIN/SCO...1,3,5-cycloheptatriene...
[spelling error]

273 **9. Bibliography**
59SCO/DOU Scott, D.W., Douslin, D.R., etc.
[reference entered twice]

274 **9. Bibliography**
Incorrect 59WES ...in simmetrical molecules...
Correct 59WES ...in symmetrical molecules...
[spelling error]

275 **9. Bibliography**
Incorrect 62SCO/GOO...J. Chem. Phys. **26**, 406-412 (1962).
J. Chem. Phys. **36**, 406-412 (1962).
Correct 62SCO/GOO...J. Chem. Phys. **36**, 406-412 (1962).
[double citation of journal with errors]

275 **9. Bibliography**
Incorrect 62SCO/MES...4-Fluortoluene:...
...J. Chem. Physa. ...
Correct 62SCO/MES...4-Fluorotoluene:...
...J. Chem. Phys. ....
[typographical errors]

275 **9. Bibliography**
Incorrect 63HUT/COL...L-laucine...
Correct 63HUT/COL...L-leucine...
[typopgraphical error]

277 **9. Bibliography**
Incorrect 66GEL Geller, B.E., Some physicochemical properties of dimethylformamide,
Zhur. Fiz. Khim. **40**, 1956-1958 (1966).
Correct 61GEL Geller, B.E., Some physococochemical properties of dimethylformamide,
Zhur. Fiz. Khim. *35*, 2210-2216 (1961).
[reference error]

277 **9. Bibliography**
Incorrect 66ZAL/STR...Zalikin, and A.A., Strepikheev, Yu.A.,...
Correct 66ZAL/STR...Zalikin, A.A., and Strepikheev, Yu.A.,...
[typographical error]

278 **9. Bibliography**
Incorrect 68GEE/MEL...Makroknol. Chem. ...
Correct 68GEE/MEL...Makromol. Chem. ...
[typographical error]

278 **9. Bibliography**
Incorrect 68WES/WUL Westrum, E.F., Jr., and Wulff, C.A.,...
Correct 68GIR/WES Girdhar, H.L., Westrum, E.F., Jr., and Wulff, C.A.,...
[author citation error]

278 **9. Bibliography**
Incorrect 69HUT/COL...bovine chymotripsinogen...
Correct 69HUT/COL...bovine chymotrypsinogen...
[typographical error]

279 **9. Bibliography**
Incorrect 70TAK/WFS Takahashi, Y., and Westrum, E.F., Jr.,...
Correct 70TAK/WES Takahashi, Y., and Westrum, E.F., Jr.,...
[typorgaphical error]

280 **9. Bibliography**
Incorrect 73AND/MAR...Part II. ...
Correct 73AND/MAR...Part 11. ...
[eleven, not Roman II]

281 **9. Bibliography**
Incorrect 73KUS/SUU...and Wadso, Thermochemistry of ...
Correct 73KUS/SUU...and Wadso, I., Thermochemistry of...
[first name initial omitted]

282 **9. Bibliography**
Incorrect [reference missing]
Correct 75LEB/TSV Lebedev, B.V., Tsvetkova, L. Ya., Kirparisova, E.G., and Lebedev, N.K., Thermodynamic properties of cycloocta-1,5-diene, Zhur. Fiz. Khim. **49**, 2152 (1975).
[reference omitted]

284 **9. Bibliography**
Incorrect 79LEB/LIT...264–265 (1979).
Correct 79LEB/LIT...364–365 (1979).
[numerical error]

284 **9. Bibliography**
Incorrect 79PUC/PEA Fuchs, R., and Peabody, L.A.,...
Correct 79FUC/PEA Fuchs, R., and Peabody, L.A.,...
[typographical error]

285 **9. Bibliography**
Incorrect [reference missing]
Correct 80WON/WES Wong, W.K., and Westrum, E.F., Jr., Thermodynamics of polynuclear aromatic molecules. II. Low temperature thermal properties of perylene, coronene, and naphthacene, Mol. Cryst. Liq. Cryst. **61**, 207-228 (1980).
[reference omitted]

285 **9. Bibliography**
Incorrect 81LEB/YEV 2 ...Kiparisova, Y.E.,...
Correct 81LEB/YEV 2 ...Kiparisova, Y.G.,...
[spelling error]

286 **9. Bibliography**
Incorrect 81TOM/CUR ...1,1'-dibenzolferrocene...
Correct 81TOM/CUR ...1,1'-dibenzoylferrocene...
[spelling error]

286 **9. Bibliography**
Incorrect 82MOR/MAT ...cryo-refigerator...
Correct 82MOR/MAT ...cryo-refrigerator...
[spelling error]

286 **9. Bibliography**
Incorrect 82SCH/MIL 2 ...II. Molar heat of seven...
Correct 82SCH/MIL 2 ...II. Molar heat capacities of seven...
[word omitted]

286 **9. Bibliography**
82WIL/ING
[out of place alphabetically].