Heat Capacities of Organic Compounds in the Liquid State
I. C_1 to C_{18} 1-Alkanols

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Heat capacities of liquid C_1 to C_{18} 1-alkanols measured by calorimetric methods were compiled and evaluated. The selected experimental data were fitted as a function of temperature with cubic splines using weighted least squares minimization. The parameters of the cubic spline polynomials and the recommended values for heat capacities are presented. A new quasi-polynomial equation which permits extrapolation of heat capacities outside the temperature range of experimental values was derived and its parameters for C_1 to C_{10} 1-alkanols are presented.

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1. Introduction

Detailed information on thermophysical and equilibrium thermodynamic data for the important homologous series of organic compounds is of both theoretical and practical interest. The Subcommittee on Thermodynamic Data of the IUPAC Commission on Thermodynamics recently initiated several international data projects. The main purpose of these projects is to stimulate world wide cooperation of experimentalists and data evaluators, in order to establish representative and consistent data bases of evaluated data on different thermodynamic properties.

This article was prepared in connection with the IUPAC projects "The Vapor-Liquid Equilibria in 1-Alkanol + n-Alkanes Mixtures" and "The Heat Capacities of Liquid Substances". The main objective of this critical compilation is to review and evaluate all calorimetric data on heat capacities of 1-alkanols up to C_{18} in the liquid state, and to present the "best" recommended values obtained by temperature correlation of the data from the selected sources.

1.1. Previous compilations

Although attention has been paid over the last 20 years to the evaluation of thermodynamic properties of alcohols, there is no current critical compilation which would present temperature correlation of critically reviewed heat capacity data for the homologous series of 1-alkanols. New important measurements were pub-

lished recently (most of the data for C_{10} and higher 1-alkanols appeared within the last 10 years) and older evaluations need an updating.

Touloukian and Makita (70TOU/MAK) compiled and evaluated heat capacity data for 55 industrially important pure substances, including methanol and ethanol. As important new measurements were carried out for both alkanols in the meantime, their evaluation is not up-to-date anymore. In the Supplement to this compilation (76TOU/MAK) some other alcohols are included; the data were not, however, critically assessed and no recommendations were given.

The physicochemical data for aliphatic alkanols are summarized in a compilation by Wilhoit and Zwolinski (73WIL/ZVO); an overview of heat capacity sources is given but recommended values are presented only at one or more of three typical temperatures (melting point, normal boiling point, 298.15 K).

The most recent Soviet compilation of thermodynamic properties of oxygen containing organic compounds (84VAS/PET) also summarizes the data from the sources which are not readily available in the West. However, only the raw data from different sources are tabulated (with the estimation of their accuracy) without any comparison, correlation and recommendation.

An impressive amount of data sources is listed in the compilation of thermodynamic properties of organic compounds, in the condensed state, by Domalski and coworkers (84DOM/EVA). Heat capacity with the general evaluation of accuracy is given usually only at one temperature for each listed reference, no recommended values were generated.

Wilhoit et al. (85WIL/CHA) published a very thorough evaluation and correlation of heat capacity data in condensed phases for oxygen containing compounds C_1 to C_4. Their recommendations for the four lowest members of the homologous series of 1-alkanols are updated by this article as we include some recent sources which were not considered by them.

Two recent evaluations published in "non-open" literature are the recommended heat capacities for the liquid 1-alkanols C_1 to C_5 tabulated by the Thermodynamics Research Center of Texas A&M University (87TRC) and the recommended data generated for saturation heat capacities of aliphatic alcohols C_1 to C_{16} by the Engineering Science Data Unit (79ENG). In the latter report parameters of temperature correlation and recommended values are tabulated for the temperature range between melting point temperature and 320 to 400 K according to the type of the substance. Data sources which were used to establish the equations are listed, but no details about the assessment and selection process are given; for certain compounds where little experimental data were available the parameters were estimated.

Heat capacity data for 1-alkanols are also listed in a number of general tables of physicochemical properties; the most important of them are reviewed by Wilhoit et al. (85WIL/CHA). Either direct experimental or smoothed values are tabulated; although in most tables

the references to the used data sources are presented, there is not usually any other specification available.

1.2. Types of Heat Capacity Data

Thermodynamics defines three types of heat capacities: isochoric, isobaric and saturation. While the first type is rarely determined experimentally for liquids, and is primarily of theoretical interest, the data for the other two heat capacities are reported in the literature. Isobaric heat capacity is defined as

$$C_p = T(\partial S/\partial T)_p = (\partial H/\partial T)_p \qquad (1)$$

and saturation heat capacity as

$$C_{sat} = T(\partial S/\partial T)_{sat} \qquad (2)$$

where subscript sat denotes that pressure changes with temperature along the vapor-liquid saturation curve.

In most experimental determinations, a sample under investigation is heated or cooled; the amount of exchanged heat and the corresponding temperature change are measured. When the process is carried out at constant pressure, the isobaric heat capacity C_p is obtained. If the temperature change is performed under conditions of vapor-liquid equilibrium, the experimental value is saturation heat capacity C_{sat}. In this case the heat capacity of a two phase system is measured. This quantity has to be converted to C_{sat} using correction for heat capacity of vapor and enthalpy of vaporization which both contribute to the total value of the measured heat (46HOG).

Heat capacities are related by definition to temperature derivatives of entropy, and the experimental values corresponding to finite temperature change cannot be automatically considered as C_p and C_{sat} defined by Eqs. (1) and (2). The heat capacity of organic liquids changes moderately with temperature (except in the region of high vapor pressures) and the true heat capacity equals in most cases the experimental value within the error of measurement if the temperature increment does not exceed several degrees (temperature changes between 3 to 8 K are the most frequent). When the temperature change in the experiment is above 10 K, the value obtained is denoted in the following tables as average heat capacity C_{avg}. This type of quantity has never been used for establishing recommended values.

Below the normal boiling temperature the experimental isobaric heat capacity usually relates to the atmospheric pressure though it is not frequently specified in the original source. C_p depends little on pressure at low and moderate vapor pressures, and its effect can be neglected unless the pressure change is large. Above the normal boiling temperature the saturation heat capacities rather than C_p data are reported in the original literature. Measurements with pure 1-alkanols at pressures remote from the vapor pressure are rare; they are interesting primarily for mixture investigation and no special atten-

tion has been paid to them in the context of this compilation. These data were considered (after the appropriate correction) only as exceptions in those cases when they were determined at pressures not too far removed from the saturation line and they extended the temperature range of available data.

The relationship between saturation and isobaric heat capacities can be derived from the entropy differential expressed as a function of temperature and pressure. The final equation connecting C_{sat} and C_p at the same temperature T and vapor pressure p_{sat} is:

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

The conversion can be made using temperature correlations of liquid density and vapor pressure. Both derivatives in Eq. (3) are positive and C_{sat} is therefore always smaller than C_p. The second term on the right hand side of Eq. (3) increases with increasing vapor pressure and becomes important only at temperatures far above the normal boiling point temperature T_b. Below that temperature the difference between C_p and C_{sat} is substantially smaller than the uncertainty in very precise heat capacity measurements (0.1 percent).

In the cases where heat capacities are tabulated in this article above the normal boiling temperature, they always relate to the vapor pressure of the compound. Both types of heat capacity are tabulated only in those cases when the difference between C_p and C_{sat} is not substantially smaller than the error of experimental data; conversions were carried out using Eq. (3). As there are not enough data on expansivities of alkanols, the term $(\partial V/\partial T)_p$ was approximated by $(\partial V/\partial T)_{sat}$ (except for methanol, see Sec. 3.1.); the difference between them becomes important only far above the normal boiling temperature. The latter term was calculated from the temperature correlation of densities along the saturation line using a modified Rackett equation (85CAM/THO) or the Francis equation (86SMI/SRI). The derivative $(dp/dT)_{sat}$ was calculated from the Wagner or Antoine vapor pressure equations (references 83MCG and 79DYK/REP, respectively).

The conversion was performed only at temperatures higher than $0.9T_b$ for C_1 to C_4 1-alkanols where both types of heat capacities are tabulated. No distinction between these heat capacities was made for other 1-alkanols (see Sec. 4. for details). The symbol C without a subscript specification or the term heat capacity are used throughout this paper whenever we refer both to C_p and C_{sat} or when the difference between their values for particular conditions is negligible compared to the expected experimental error.

1.3. Characterization of calorimetric techniques for determining heat capacities of liquids

The experimental methods used in determination of heat capacities of liquids are briefly outlined below. This survey is included to explain the meaning of abbreviations used in tables of experimental heat capacities (see Sec. 4.1. for a detailed description of the Tables).

AD — adiabatic calorimetry. A sample is placed inside a calorimetric vessel (provided with a thermometer and a heater) which is fully surrounded by a heated jacket. Its temperature follows exactly that of the vessel in order to avoid any transfer of heat between the vessel and its surrounding. The heat capacity is calculated from the measured amount of the electric energy supplied to the vessel and the corresponding increase in its temperature. No calibration is necessary, but corrections for small deviations from the strictly adiabatic regime are usually needed.

CC — measurement of cooling curve. A sample is heated and then placed into a thermostat whose temperature (lower than that of the substance) is maintained constant. The time taken to cool the sample is proportional to the heat capacity of the sample. The method is comparative, measurement with a reference substance of a well defined heat capacity has to be performed under the same conditions.

CT — use of the Calvet-Tian type of calorimeter. Two identical vessels (filled with studied and reference substances) are connected with thermopiles and placed inside a massive metallic block. When the same amount of heat is introduced into both vessels, a temperature imbalance between them occurs due to different heat capacities of the substances. The resulting temperature difference is eliminated by a heat flow through the thermopiles reflected in an electric signal which is proportional to the difference in heat capacities of the samples. The most common instruments of this type are French commercial calorimeters by SETARAM.

DC — differential calorimetry. The same amount of heat is introduced into two thermostatted calorimetric vessels filled with a studied and reference material. The heat capacity is calculated from the temperature difference between the two vessels. The Calvet-Tian calorimeter is a special type of this apparatus.

DR — drop calorimetry. An ampoule with a sample is heated to a well defined temperature and dropped into a surroundings at the lower temperature. In the simplest version of the method, the increase in temperature of a Dewar flask filled with water is measured after dropping a sample (most heat capacities were determined in this way in the 19th century). More accurate results are obtained in an isothermal arrangement where volume change during a phase transition induced by cooling of the sample is measured (e.g. melting of ice in Bunsen ice calorimeter). This technique always leads to average heat capacity C_{avg}.

DS — differential scanning calorimetry. It is a special type of differential calorimeter where both vessels (containing a sample and a reference substance) are continuously heated; the electric inputs to the heaters of the vessels are automatically adjusted to keep a constant rate of temperature increase in both vessels. The difference in power supplied to the vessels is proportional to the difference in heat capacities.

FL — flow calorimetry. A liquid under investigation flows at a constant rate through a heated tube, and the increase in temperature of the substance is measured. Volumetric heat capacity is obtained from the flow rate, electrical input and the difference in temperature of liquid after and before heating. Density of sample has to be available for conversion to the heat capacity per mole or unit mass. This principle is used in the Picker differential flow calorimeter which is available commercially (SETARAM, SODEV). The instrument works on the principle of a thermal balance. Studied and reference liquids enter the measuring cells at the identical temperature and the heating inputs are automatically adjusted to give the same temperature increase. The serial connection of the cells provides for reduction of noise from flow rate fluctuations.

IP — isoperibol calorimetry. The calorimetric vessel (provided with a heater and a thermometer) is insulated from the surroundings which is maintained at a constant temperature — a Dewar flask in a thermostatted room is the simplest arrangement. The amount of electric energy needed to increase the temperature of the vessel by several degrees is measured. Calibration with a reference material is needed in order to get a reasonable accuracy.

RP — regular pulsing technique. A cylindrical calorimetric vessel is filled completely with a sample. A narrow tube with a heating wire at its center passes through the vessel along its axis. Periodically either electric pulses are supplied to the heater or the cooling agent is passed through the tube. Heat capacity and thermal conductivity can be obtained from the measured oscillations of temperature in the vessel. This rapid but not too accurate method (experimental error 2 to 3 percent) was used primarily in the Soviet laboratories.

2. Methodology of Establishing the Recommended Data

2.1 Evaluation and Selection Process

Experimental heat capacities along with auxiliary data extracted from original sources were stored in a database of raw data. The auxiliary data comprised information on the nature of experimental procedure, sample purity and quality of experimental values. This information was used as a guide in the selection of data sets for establishing the recommended values; all available sources were critically assessed. The important part of the selection process was the simultaneous correlation of all experimental data which served to test the consistency and helped to reveal the systematic errors. The correlation was performed by the weighted least-squares method; the minimized objective function S had the form

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

where the summation is over all the values included in the correlation and subscript "exp" and "sm" relate to experimental and smoothed values, respectively. The reciprocal of the variance $\sigma^2(C)$ has the meaning of the weighting factor. It was estimated for each value on the basis of the assumed experimental error of the data set used in the correlation. The input information was the percentage error of experimental data, $\sigma_r C$, as given by the author for the whole data set or estimated by the compiler. Thus the variance of the i-th data point was expressed as:

$$\sigma^2(C)_i = [(C)_i . \sigma_r C / 100]^2 \qquad (5)$$

The following criteria were observed in the selection process:
1. Accuracy of the measurement claimed by the author;
2. Reputation of the laboratory and credibility of the author's measurements;
3. Consistency of the data with the values from other sources (if available);
4. Purity of the substance;
5. Type of the calorimeter;
6. Time of data origin (measurements published after the year 1940 were preferred); and,
7. Scatter of the data

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

(a) All available heat capacity data sets along with the information on their accuracies were read in and after conversion to the same type of heat capacity (C_1 to C_4 1-alkanols) a preliminary joint correlation was performed. Prior to the correlation, data sets considered a priori as unreliable were discarded if more accurate data were available for the same temperature range. For those sources where only parameters of a smoothing equation were available, pseudo-discrete data were generated in the temperature range of the parameters' validity. A temperature step of 5 to 10 K was used according to the length of the temperature interval and density of data points from other sources.

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

(c) The correlation was repeated several times until the final fit with the selected data was obtained

where differences between experimental and smoothed values were roughly equal to or smaller than expected experimental errors. The final correlation of the selected experimental data was assigned a level of accuracy (I to VI) according to the quality of the correlated data.

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

$$s_w = [S_{min}/(n-m)]^{1/2} \qquad (6)$$

where n is the overall number of the fitted data points and m is number of independent adjustable parameters in a correlation equation. When experimental data are consistent within the expected error limits, s_w should be close to unity. In addition, use of the following statistical criteria was made:
the standard deviation

$$s = \{[\sum_{i=1}^{n}(C_{sm}-C_{exp})_i^2]/(n-m)\}^{1/2} , \qquad (7)$$

the percentage standard deviation

$$s_r = \{[\sum_{i=1}^{n}((C_{sm}-C_{exp})/C_{exp})_i^2]/(n-m)\}^{1/2}\cdot100 , \qquad (8)$$

the bias

$$s_b = [\sum_{i=1}^{n}(C_{sm}-C_{exp})_i]/n. \qquad (9)$$

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

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

the average weighted deviation

$$d_w = \{[\sum_{i=1}^{n_1}((C_{sms}-C_{exp})^2/\sigma^2C^1)_i]/n_1\}^{1/2} , \qquad (10)$$

the average deviation

$$d = \{[\sum_{i=1}^{n_1}(C_{sm}-C_{exp})_i^2]/n_1\}^{1/2} , \qquad (11)$$

the average percentage deviation

$$d_r = \{[\sum_{i=1}^{n_1}((C_{sm}-C_{exp})/C_{exp})_i^2]/n_1\}^{1/2}\cdot100 , \qquad (12)$$

the bias of a data set

$$d_b = [\sum_{i=1}^{n_1}(C_{sm}-C_{exp})_i]/n_1 \qquad (13)$$

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

2.2. Correlation Equations

When examining the possible approaches to the temperature correlation of heat capacity data, two main criteria were considered:

1. The ability to fit precisely the selected experimental data over the whole temperature range with a relatively small number of parameters.

2. The possibility of a meaningful extrapolation above the upper temperature limit of experimental data.

A polynomial equation appears to be the most dependable in describing heat capacity as a function of temperature and has been used for description of C_p or C_{sat} of alcohols in most previous compilations (70TOU/MAK, 85WIL/CHA) where the parameters of the regression equation were listed. The temperature dependence of the heat capacity for 1-alkanols is rather complex and a polynomial of up to the eighth degree might be needed in cases where data are available over a wide temperature range. The substantial drawback of the polynomials of a high degree is a possibility of oscillation and ill conditioning of parameters. We preferred to fit the selected experimental values with cubic splines which proved to be useful in describing complex functions in a number of technical applications.

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

When using cubic splines for smoothing experimental data the knot temperatures have to be chosen first and then the heat capacity values at knots are adjusted by a spline correlation routine in order to minimize the objective function S defined by Eq. (4). We used the correlation algorithm developed at the Technical University of Budapest (79KOL) in which the two boundary conditions are considered during minimization as two additional adjustable parameters. Three to four knots (i. e. five to six independent parameters) were necessary for the satisfactory fit of the data for 1-alkanols within the expected experimental errors.

The results of spline correlation are usually reported in terms of the knot values and two boundary conditions;

the spline routine is then necessary for generating the recommended data. As we expect that this routine is not available to all users of the data we preferred to tabulate directly the parameters of cubic polynomials which are easier to use. A single polynomial linear in temperature was used for one compound where data were available in a limited temperature range only. The adjustable parameters A_j relate to the equation

$$C/R = \sum_{j=0}^{m} A_j(T/100)^j, \qquad (14)$$

where R is the gas constant. The upper limit of the summation m is equal to 3 in all cases where the overall temperature range is subdivided (cubic splines fitting) or can be lower when only one polynomial is used to describe the data. Dividing temperature by a scaling factor of 100 improved the numerical stability of the set of normal equations used in determining the parameters.

The cubic splines are very flexible when describing the temperature dependence of heat capacity inside the limits of the temperature range of experimental data, i.e. they are excellent for interpolation. However, the cubic splines cannot be used for a meaningful extrapolation. Thus, another correlation equation was proposed which should provide for a reasonable extrapolation, especially towards the critical point. The derivation of this new relationship — further denoted as "quasi-polynomial equation" — is based on the assumption that the heat capacity of most organic liquids is an increasing function of temperature. The only exceptions occur for a few substances which show a shallow minimum a few degrees above the triple point. Such behavior is only observed with precise measurements. As the quasi-polynomial equation is aimed primarily at applications where emphasis on the extrapolation capability rather than on a perfect fit of experimental data, the possible presence of a minimum in the heat capacity curve was ignored.

Consider that the first derivative of heat capacity with respect to variable $\tau = 1 - T/T_c$ is a quadratic function of the form

$$dC/d\tau = - (e_{-1}/\tau + e_1\tau + e_2\tau^2)^2 \qquad (15)$$

where e_{-1}, e_1, e_2 are adjustable parameters. After integration one obtains

$$C = e_{-1}^2/\tau + e_0 - 2e_{-1}e_1\tau - e_{-1}e_2\tau^2 -$$

$$e_1^2\tau^3/3 - e_1e_2\tau^4/2 - e_2^2\tau^5/5 \qquad (16)$$

where e_0 is an adjustable parameter resulting from integration. Due to the form of Eq. (15), $dC/d\tau$ is always negative and the dC/dT must be always positive; therefore the right hand side of Eq. (16) is an increasing function of temperature. The term e_{-1}^2/τ provides for a sharp increase of heat capacity as the critical point is approached. This is in agreement with the theory of liquid state which predicts C_p and C_{sat} to be unbounded at T_c. Equation (16) can be modified to give a power series in τ

$$C/R = \sum_{i=-1}^{m} E_i\tau^i \qquad (17)$$

where E_i are parameters related to the coefficients e_i in Eq. (16) and the upper limit of summation m equals 5.

2.3. Units, Conversion Factors, Temperature Scales

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

1 cal = 4.1840 J
1 Btu lb^{-1}($^{\circ}$F)$^{-1}$ = 4.1868 J K^{-1}g^{-1}
$T/K = T/^{\circ}C + 273.15$
$T/K = 0.55555\ T/^{\circ}F + 255.37$
$R = 8.31441$ J K^{-1}mol^{-1}.

Molar masses were calculated from atomic masses recommended by the IUPAC Commission on Atomic Weights (84COM). The differences in temperature scales were neglected for two reasons. First, the highest relative error in heat capacity introduced by neglecting the difference between IPTS-68 and IPTS-48 temperature scales was in the range 10^{-4} to 10^{-5} percent which is several orders of magnitude smaller than the precision of the best heat capacity measurements. Second, it was not clear in some cases, particularly for older measurements, which temperature scale was adopted by the author.

3. Heat Capacity Data on 1-Alkanols — Availability, Consistency and Temperature Dependence

The literature search was limited to sources published after 1920. Only calorimetric measurements of heat capacities were compiled (see the brief characterization of experimental methods in Sec. 1.3.). Neither enthalpic measurements on reference-fluid boil-off calorimeters nor heat capacities determined by indirect techniques (compressibility and piezothermic methods) were considered.

The substantial part of heat capacity data discussed below are sub or superambient measurements carried out usually on adiabatic heat capacity calorimeters over a considerable temperature range. Near ambient conditions, the measurements performed over a limited temperature range or at one temperature only (usually at 298.15 K) are common for C_1 to C_6 1-alkanols. The latter data were typically determined during thermodynamic investigation on mixtures, as the values at the limit of a concentration range.

We did not pay special attention to the problems of solid-liquid phase transition for 1-alkanols; some compounds tend to form glasses and their melting points are not well defined. More information can be found in the literature (73WIL/ZVO, 85WIL/CHA).

3.1. Selection of Data for C_1 to C_5 1-Alkanols

The experimental heat capacities on C_1 to C_5 1-alkanols are abundant and several sources cover relatively wide temperature ranges with good accuracy. The substantial part of the selected temperature dependent data were from four well-known laboratories which have been engaged in the heat capacity measurements for many years:

The Division of Chemical Standards of the National Physical Laboratory, Teddington, England (Counsell, Hales, Lees and Martin), data for C_3 to C_5 1-alkanols (65COU/HAL, 68COU/LEE).

The National Bureau of Standards, (Fiock, Ginnings and Holton), old but reliable data for methanol and ethanol extending above the normal boiling temperature (31FIO/GIN).

The Department of Chemistry, University of Michigan, Ann Arbor, Michigan (Carlson and Westrum), data for methanol (71CAR/WES)

The Department of Chemistry, University of Osaka, Toyonaka, Osaka (Haida, Suga and Seki), data for ethanol (77HAI/SUG).

Grigor'ev and coworkers (79GRI/YAN) at the Groznenskii Petroleum Institute (Groznenskii Neftyanoi Institut), USSR reported data on C_3 to C_5 1-alkanols reaching from temperatures close to ambient up to 463 K. Description of the experimental procedure is very concise and it is not quite obvious what type of heat capacity was determined. Measurements were carried out at pressures slightly above the vapor pressure and the tabulated results are claimed to be isobaric heat capacities relating to the saturation line. Although there is little information on the data in the original literature, their consistency (usually within 1 percent) with the results from other laboratories is acceptable. This is the only source reporting data for C_3 and C_5 1-alkanols above the normal boiling temperature.

The data from the above sources were complemented by measurements from other laboratories which were considered reliable, reasonably consistent and extended, in some cases, the temperature range of experimental values. In the case of ethanol these were the low temperature measurements of Ziegler and coworkers (66HWA/ZIE, 79BRO/ZIE) carried out at Georgia Institute of Technology, Atlanta, which were in excellent agreement with the Japanese results (77HAI/SUG).

Boyette and Criss (88BOY/CRI) performed measurements for methanol at 8.3 MPa up to a temperature 9 K below the critical point. The conversion to the vapor pressure had to be carried out in order to be able to include these data in our correlation. The following thermodynamic relationship was used:

$$[\,C_p\,]_{V_1}^{V_2} = T \int_{V_1}^{V_2} (\partial^2 p/\partial T^2)\, dV -$$

$$[T(\partial p/\partial T)_V{}^2/(\partial p/\partial V)_T\,]_{V_1}^{V_2} \qquad (18)$$

where the volumes V_1 and V_2 correspond to the experimental pressure and the vapor pressure p_s, respectively.

The bracketed expressions denote the difference of the given quantity between the pressures corresponding to V_2 and V_1. The equation of state for methanol by Machado and Street (83MAC/STR) was used, vapor pressures were obtained from the Wagner equation with constants determined by McGarry (83MCG). We assigned an uncertainty of $\pm 3\%$ to the corrected values. The second term on the right hand side of Eq. (3) was estimated in a similar way.

For 1-propanol we included also the values obtained at the Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw (80KAL/JED) and the measurements by Eucken and Eigen (51EUC/EIG) at the University of Göttingen. While the data from the former source were in excellent agreement with the measurements from NPL, England (68COU/LEE) there was a serious disagreement with the latter source near the lower temperature limit of the data and therefore only the values from the upper part of the temperature interval were included.

For 1-butanol above its normal boiling temperature we also considered isobaric heat capacities of San Jose (75SAN) determined at pressure near 1.4 MPa at Massachusetts Institute of Technology, USA. A minor pVT correction to convert these data from the experimental pressure to the vapor pressure was applied; its maximum value is around 0.3 percent of the heat capacity value. The data seem to be more scattered compared to those of Grigor'ev *et al.* and are in most cases lower.

In the case of C_2 to C_5 1-alkanols a number of one-temperature measurements (usually at or near 298.15 K) and some measurements in a limited temperature interval near ambient conditions (86GAT/WOO, 66KLE) were included.

Wilhoit *et al.* (85WIL/CHA) did evaluation of thermodynamic properties for C_1 to C_4 alkanols in the condensed phases. For methanol and ethanol we adopted an identical procedure for converting the experimental enthalpy data reported by Fiock and Ginnings (31FIO/GIN) to saturation heat capacities. The agreement of our recommendations with those of Wilhoit and coworkers is, for these two alcohols, within ± 0.1 percent. There are some differences for C_3 and C_4 1-alkanols, due to the fact that we included some more recent data covering a larger temperature range. For 1-propanol the agreement is within ± 0.2 percent except around the temperature 380 K where our recommendations are 0.5 percent higher. This is the region just above the upper temperature limit of the data of Counsell and Lee. Wilhoit *et al.* considered only the measurements by Eucken and Eigen which are systematically lower by several percent compared to the previous source. For 1-butanol agreement to ± 0.1 percent is observed below 320 K (region where both evaluations used measurements by Counsell *et al.*). Above this temperature our recommendations are lower (up to 0.7 percent near the upper temperature limit). Wilhoit *et al.* used old measurements (*81REI) and (24WIL/DAN) which we consider less credible than our selection (75SAN, 79GRI/YAN).

3.2. Selection of Data for C_6 to C_8 1-Alkanols

The selection of data for C_6 to C_8 1-alkanols was more complicated. Although several data sources are available for each compound, they are not generally consistent. Differences of several percent are quite common and it is hard to decide which sources should be selected for the final correlation. In order to obtain some guidance in evaluating the data sources, measurements between 298 and 318 K were carried out with all three 1-alkanols at the Institute of Chemical Technology in Prague (89VES/BAR). They made it possible to check the low temperature measurements near their upper temperature limit and the superambient data close to their lower temperature limit.

Concerning the low temperature data, only one source was available for C_7 and C_8 1-alkanols and though the data of Cline and Andrews (31CLI/AND) for 1-octanol were scattered and differed strongly near room temperature from the other sources, there was no other choice. The distortion of the heat capacity curve for 1-octanol in the low temperature range is apparent in Fig. 17. For 1-hexanol, the results of extensive measurements from the Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw (84KAL/WOY) are 2 to 5 percent higher compared to the old low temperature values of Kelley (29KEL2) and other data at ambient temperature. As the results of the same Polish authors for 1-propanol measured four years earlier on the same instrument seem to be very good, we suspect that contamination of the sample is the reason for this discrepancy. When the heat capacity versus temperature curves for C_5 to C_7 1-alkanols were compared, it was obvious that the curve for 1-hexanol would have been too high at low temperatures if the Polish data had been considered as the only source. We did not, however, reject these measurements but included them in the correlation with a lower weight (see Table 17). The reason is that we do not consider the old data by Kelley as very reliable either, and we preferred a compromise rather than using exclusively one data set in the subambient region.

The measurements at superambient temperatures are almost exclusively from the Soviet laboratories. Here again we preferred the data from Groznenskii Neftyanoi Institut, (79GRI/YAN) compared to those from other laboratories: Stepanakertskii Gosudarstvenyi Universitet, Stepanakertsk (81ARU) and Azerbaidzhanskii Politekhnicheskii Institut, Baku (86NAZ/BAS2, 88NAZ/BAS).

3.3. Selection of Data for C_9 to C_{18} 1-Alkanols

The amount of information and credibility of data on higher 1-alkanols decrease with increasing length of the carbon chain. Consistency of data from different sources is generally poor and it is sometimes difficult to decide which data sets should be selected. Only one literature source was found for 1-hexadecanol and no measurements at all were reported for 1-heptadecanol.

First of all, the Soviet laboratories carried out extensive investigations on higher members of this series. For C_9 and C_{10} 1-alkanols we selected, as for the lower 1-alkanols, the data of Grigor'ev et al. (79GRI/YAN). For the C_{11} and higher 1-alkanols (with the exception of 1-dodecanol) the measurements of Vasil'ev, Petrov and coworkers (80VAS/TRE, 82VAS/PET) from the Soviet Research Institut of Petroleum Chemistry (Vsesoyuznyi Nauchno-Issledovatel'skii Institut Neftekhimicheskikh Protsessov), in Leningrad were the only source of data over the large temperature range. Only parameters of polynomials describing heat capacity as a quadratic function of temperature in several subintervals are given in the latter source. When plotting the data generated from these polynomials we observed a strong discontinuity of the first derivative at the limits of the subintervals. There is probably something wrong with the experimental values (which are not accessible) or with the correlation. There seems to be even a shallow minimum on the heat capacity curve at high temperatures.

The only western C_p measurements over a wide temperature range are those of Svensson (79SWE) performed on a commercial DSC calorimeter for C_{10} and C_{12} 1-alkanols at the Thermochemistry Center of the University of Lund, Sweden. They suggest also a considerable decrease in the temperature derivative of the heat capacity as the upper temperature limit is approached. Data measured over a limited temperature range near room temperature were reported for 1-decanol by Costas and Patterson (85COS/PAT) from the McGill University in Montreal and for C_{13} and C_{16} 1-alkanols by Mosselman et al. from the Free University in Amsterdam. The latter authors give only a polynomial linear in temperature as a representation of their data.

Considering the scarcity of data sources and their poor consistency one should approach the recommended data for C_{11} and higher 1-alkanols with caution. We have developed a contribution technique (90ZAB/RUZ) for calculating liquid heat capacities of 1-alkanols. This method is based on all values resulting from this evaluation and might be useful in those cases where a uniform and consistent description of all high 1-alkanols is required.

Another problem concerns the possibility of decomposition for compounds with long carbon chains at high temperatures. Ambrose and Sprake (70AMB/SPR) found during their vapor pressure measurements that decomposition is likely to occur at temperatures above 550, 570 and 575 for C_{12}, C_{16} and C_{18} 1-alkanols, respectively. This information can serve as a guide for all high 1-alkanols. How-ever, very few heat capacity data are available above these temperature limits and we did not therefore examine more closely stability of compounds.

3.4. Temperature Variation of
Heat Capacity for 1-Alkanols

The temperature dependence of heat capacity for liquid n-alkanes is a convex function except a shallow minimum near the triple point temperature. It is often assumed that the temperature variation of liquid heat capacity for 1-alkanols should be similar. The liquid C_1 to C_3 1-alkanols actually might have a very shallow extremum in the vicinity of the lower temperature limit. There is, however, experimental evidence that the heat capacity curve for C_4 and higher 1-alkanols exhibits an inflexion point. The accurate measurements for 1-pentanol (68COU/LEE) suggested the presence of an inflexion point near the reduced temperature $T_r = 0.6$; a similar finding was reported for 1-butanol (75SAN). The recent results of Soviet authors for C_6 and higher 1-alkanols (79GRI/YAN, 80VAS/TRE, 82VAS/PET, 86NAZ/BAS2, 88NAZ/BAS) indicate a strong "flattening" of the heat capacity curves at high temperatures (especially for C_{13} and higher 1-alkanols). However, little is known about the reliability of these data and in many cases only parameters of regression polynomials are available, which prevents an evaluator from a deeper insight into the data. The heat capacity equations published for 1-alkanols in the report of the Engineering Science Data Unit (79ENG) represent C_{sat} as a convex function of temperature. On the other hand the results of our correlation combining data from several sources indicate presence of inflexion points starting with 1-propanol. To prove the systematic presence of inflexion points and to demonstrate shifts in their location with the increasing length of the carbon chain would require additional accurate measurements over a considerable temperature range for several members of the homologous series (especially for higher 1-alkanols). This feature of the temperature dependence of C for 1-alkanols can be explained by the presence of hydrogen-bonded clusters which tend to break up as temperature is increased. These changes in the structure of the liquid are reflected sensitively in the temperature variation of heat capacity. The plot of saturation heat capacity versus temperature is given for C_1 to C_8 and for C_9 to C_{18} 1-alkanols in Figs. 17 and 18, respectively.

lists in the upper half sources selected for establishing the recommended values; the statistical criteria defined in Sec. 2.1. indicate for both selected and discarded sources how the individual data sets compare with values generated from the correlation equation. The data consistency is well demonstrated in the deviation plots (Figs. 1 to 15). Tables listing parameters obtained from the spline correlation of the selected data also give information on the quality of the overall fit and reliability of the recommended data.

Recommended values generated from the cubic splines and parameters of quasi-polynomial extrapolation Eq. (17) are tabulated together for all 1-alkanols in Tables 51 and 52, respectively. Graphical representation of the recommended data is in Figs. 17 and 18 at the end of the article.

Correlations for both isobaric and saturation heat capacities were performed for C_1 to C_4 1-alkanols. No distinction is made between the two heat capacities for C_5 and higher 1-alkanols (the discussion of heat capacity types is given in Sec. 1.2.). The reasons are as follows. For C_8 to C_{18} 1-alkanols the upper temperature limit of experimental data is always below or very close to the normal boiling point temperature. The difference between C_p and C_{sat} is therefore one order of magnitude smaller compared to the error of the data. For C_5 to C_7 1-alkanols the data extend above the normal boiling temperature and the maximum difference between C_p and C_{sat} is 1.1 J $K^{-1}mol^{-1}$ (for 1-hexanol at its upper temperature limit). For these three compounds the only source of experimental data above the normal boiling temperature are the measurements of Grigor'ev and coworkers (79GRI/YAN). The accuracy of the data is around 1 percent and it is not quite clear what type of heat capacity they actually measured. For these reasons we preferred not to give any specification regarding the heat capacity type.

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

4. Description of Tables
and Deviation Plots

Most of the information on the data and their processing is given in tables which are described in detail below. The characterization of raw data, their consistency, and results of correlation are summarized for each 1-alkanol separately in three tables and a deviation plot. Tables of experimental heat capacities review all primary sources and characterize briefly experimental conditions and quality of data. The table of correlated heat capacities

4.1. Experimental Heat Capacities

Each line of the table contains information on one literature source of experimental data; when several distinct data sets were given for the same compound in one publication (parameters of smoothing equations relating to different temperature subintervals for higher 1-alkanols) there are several lines for one data source, each relating to one data set.

First column: the abbreviated reference in the form YYAAA/BBBM where YY are the last two digits of the year of publication (for a year before 1900 the reference

code is preceded by an asterisk), AAA and BBB are the first three letters of the last name of the first and second author (if present), respectively. M is a digit from 1 to 9 distinguishing papers published by the same author(s) within the same year.

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

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

Third column: number of experimental data points; symbol "eqn" is used in those cases where only parameters of a smoothing equation were presented in the original literature.

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

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

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

Seventh column: type of the calorimetric method used for determining the data and reference to the publication where the instrument is described. The abbreviations used in the table to characterize the experimental techniques are explained in Sec. 1.3.

4.2. Correlated Heat Capacities

This table contains information on the results of the correlation presented for the individual data sets. The statistics for the selected and rejected data sets are listed in the upper and lower half of the table, respectively. This table is not presented in the case of 1-hexadecanol where only one data set was available. The meaning of the columns in the upper part of the table (selected values) is as follows.

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

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

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

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

Fourth column: percentage error $\sigma_r C$ used in Eq. (5) to estimate the variance of individual data points. This value is either equal to $\sigma_r C_{exp}$ (col. 4 in the table of experimental heat capacities) or is assigned by the evaluator in cases when no specification is given in the original source or the author's estimate does not seem to be realistic. When the percentage error $\sigma_r C$ was assigned or modified by the evaluator, the value is followed by the pound sign (#).

Fifth column: average weighted deviation d_w defined by Eq. (10).

Sixth column: average deviation d (defined by Eq. (11)) divided by gas constant R (dimensionless).

Seventh column: average percentage deviation d_r defined by Eq. (12).

Eighth column: bias of the data set d_b (defined by Eq. (13)) divided by gas constant R (dimensionless).

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

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

In the case of C_1 to C_4 1-alkanols the correlations for isobaric and saturation heat capacities were performed separately. We give, however, for these compounds only one table of correlated heat capacities as the selection of data sources did not differ and values of statistics were practically identical in both correlations.

4.3. Parameters of Cubic Spline Polynomials

This table gives for each 1-alkanol in the upper part characteristics of the final correlation of the selected data and lists in the lower part the corresponding parameters of the cubic spline polynomials.

The upper part consists of two lines when both isobaric and saturation heat capacities are tabulated (C_1 to C_4 1-alkanols) and of only one line when no distinction is made between the two heat capacities (C_5 and higher 1-alkanols). The following items are listed.

First column: type of heat capacity listed — C_p and C_{sat} denote isobaric and saturation heat capacities, respectively. Symbol C is used when it was not reasonable to make any distinction between the two types of heat capacities.

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

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

Fourth column: standard weighted deviation s_w defined by Eqs. (4) and (6).

Fifth column: standard deviation s (defined by Eq. (7)) divided by gas constant R (dimensionless).

Sixth column: standard percentage deviation s_r defined by Eq. (8).

Seventh column: bias s_b (defined by Eq. (9)) divided by gas costant R (dimensionless).

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

The parameters of polynomials describing individual subintervals of the temperature range of the selected data are listed in the lower part of the table. For C_1 to C_4 1-alkanols two sets of parameters are listed separately, the first relating to the temperature correlation of C_p and the second to that of C_{sat}. The meaning of the individual columns is as follows:

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

Second to fifth columns: parameters of the cubic spline polynomial defined by Eq. (14) valid in the given subinterval. Dimension of parameters is $1/T^j$. Parameters for two to three subintervals are given except for 1-hexadecanol where the only literature source available contains parameters of a linear equation which are directly listed in the table.

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

I — excellent data (uncertainty below 0.1 percent)

II — highly reliable data (uncertainty below 0.25 percent)

III — reliable data (uncertainty below 0.5 percent)

IV — medium quality data (uncertainty below 1 percent)

V — data of low reliability (uncertainty below 3 percent)

VI — very unreliable data with a possibility of gross systematic errors (uncertainty above 3 percent).

The level of accuracy assigned to individual subintervals often differs due to the unequal reliability of experimental data in different parts of the temperature range. The lower accuracy for the high 1-alkanols in the upper temperature subinterval reflects the possibility of decomposition.

4.4. Recommended Values of Heat Capacities

Table 51 lists recommended heat capacities generated from the parameters of cubic spline polynomials at typical temperatures 273.15 and 298.15 K, and with the step 10 K over the whole temperature range of the selected experimental data. Both isobaric and saturation heat capacities are tabulated for C_1 to C_4 1-alkanols, no distinction between the two types of heat capacity is made for higher 1-alkanols. For C_{13} and higher 1-alkanols the heat

capacity is practically constant over a temperature interval of several degrees near the upper temperature limit of the data. This is caused by a peculiar character of the Soviet data (80VAS/TRE, 82VAS/PET, see Sec. 3.3. for more details). They were difficult to fit; varying position and number of knots have never prevented their oscillation around the data generated from the cubic splines (see the deviation plots). As other independent studies are not available at the same conditions it is difficult to judge if this particular variation of the heat capacity is real (see also Fig. 18).

4.5. Parameters of Quasi-Polynomial Extrapolation Equation

The quasi-polynomial equation (17) permits semiquantitative extrapolation outside the temperature range of experimental values and obeys the condition of infinite heat capacity at the critical temperature (see Sec. 2.2. for details). Parameters are given for C_1 to C_{10} 1-alkanols in Table 52. This type of correlation was not carried out for higher 1-alkanols which decompose near the upper temperature limit of the experimental data. The parameters represent C_p for C_1 to C_4 1-alkanols; no distinction between the types of heat capacity is made for higher 1-alkanols. The tabulated items have the following meaning.

First line: name of 1-alkanol.

Second line: critical temperature in kelvins.

Third to ninth line: dimensionless parameters of Eq. (17).

Tenth line: the standard deviation of the fit s (defined by Eq. (7)) divided by gas constant R.

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

4.6. Deviation Plots

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

5. Tables

TABLE 1. Experimental heat capacities for methanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type—Reference
25DRU/WEI		293.1	1	nosp	not specified	C_p	IP– 25DRU/WEI
25PAR		188.4–290.1	8	0.50	not specified	C_p	IP– 25PAR
29KEL1		181.1–292.0	14	1.00	not specified	C_p	IP– 29KEL1
29MIT/HAR		190.5–264.8	18	nosp	not specified	C_p	IP– 29MIT/HAR
31FIO/GIN	N	318.1–378.1	7	0.10	99.97 estim	C_{sat}	IP– 31FIO/GIN
39PHI		300.8	1	nosp	not specified	C_p	IP– 49WEI
49STA/GUP		180.0–270.0	10	0.50	not specified	C_p	AD– 49STA/GUP
49TSC/RIC2		298.1	1	nosp	not specified	C_p	IP– 49TSC/RIC1
50HOU/MAS		323.1–353.1	4	0.40	99.8 estim	C_p	AD– 50SAG/HOU
60SWI/ZIE	N	311.6	1	nosp	not specified	C_{avg}	DR– 58SWI/ZIE
62KAT		283.1–333.1	4	nosp	not specified	C_p	IP– 62KAT
66DRA/LAN	N	298.1	1	nosp	not specified	C_p	IP– 66DRA/LAN
68PAZ/REC	N	313.1	1	nosp	not specified	C_p	CT– 70PAZ/PAZ
71CAR/WES		180.0–320.0	17	nosp	99.975 melpt	C_p	AD– 53WES/HAT
71DES/BHA		298.1–318.1	3	1.00	not specified	C_p	IP– 56MUR/VAN
71GOP/GAM		308.0–333.0	eqn	1.00	not specified	C_p	AD– 71GOP/GAM
82BEN/DAR		288.1–308.1	2	nosp	not specified	C_p	FL– 71PIC/LED
82VIL/CAS		298.1	1	0.30	99.8 chrom	C_p	FL– 71PIC/LED
84ZEG/SOM		298.1	1	nosp	not specified	C_p	FL– 71PIC/LED
85COS/PAT		298.1–313.1	2	nosp	not specified	C_p	FL– 71PIC/LED
86KOR/KUK		278.0–298.0	2	0.20	not specified	C_p	AD– 83KUK/KOR
86OGA/MUR		298.1	1	0.10	not specified	C_p	FL– 85OGA
86TAN/TOY		298.1	1	0.30	99.96 anal	C_p	FL– 71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FL– 71PIC/LED
88BOY/CRI	N	393.1–503.1	5	nosp	not specified	C_p	FL– 87LAN/CRI
88OKA/OGA	N	298.1–299.1	2	nosp	not specified	C_p	FL– 85OGA

31FIO/GIN	data calculated using procedure by 85WIL/CHA
60SWI/ZIE	average value over the temperature range 294–329 K
66DRA/LAN	substance rated as pure, water content 0.08 per cent
68PAZ/REC	the same data in 70PAZ/PAZ
88BOY/CRI	original data measured at 8.3 MPa, converted to vapor pressure
88OKA/OGA	water content less than 0.083 mol per cent

TABLE 2. Correlated heat capacities for methanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
			Selected data					
31FIO/GIN	318.1–378.1	7	0.20#	1.732	3.61–2	0.35	−1.99–2	−3
71CAR/WES	180.0–320.0	17	0.10#	0.747	7.49–3	0.07	1.98–3	2
88BOY/CRI	393.1–503.1	5	3.00#	1.365	6.63–1	4.09	3.68–1	1

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
					Rejected data				
25DRU/WEI	(1.94–1,	2.06,	−1.94–1,	−1)	25PAR	(2.64–2,	0.29,	9.36–3,	4)
29KEL1	(6.35–2,	0.74,	−5.39–2,	−12)	29MIT/HAR	(2.88–1,	3.13,	2.46–1,	16)
39PHI	(6.18–1,	5.93,	6.18–1,	1)	49STA/GUP	(6.19–2,	0.71,	−4.09–2,	−4)
49TSC/RIC2	(2.43–1,	2.43,	2.43–1,	1)	50HOU/MAS	(1.01–1,	0.90,	7.32–2,	2)
60SWI/ZIE	(3.62–1,	3.73,	−3.62–1,	−1)	62KAT	(7.12–1,	6.52,	6.92–1,	4)
66DRA/LAN	(1.57–1,	1.59,	1.57–1,	1)	68PAZ/REC	(1.95–1,	1.89,	1.95–1,	1)

TABLE 2. Correlated heat capacities for methanol — Continued

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
					Rejected data				
71DES/BHA	(3.65 − 1,	3.51,	3.63 − 1,	3)	71GOP/GAM	(6.75 − 1,	6.94,	−6.63 − 1,	−3)
82BEN/DAR	(6.35 − 2,	0.64,	1.39 − 2,	0)	82VIL/CAS	(9.84 − 2,	1.00,	9.84 − 2,	1)
84ZEG/SOM	(4.43 − 2,	0.45,	4.43 − 2,	1)	85COS/PAT	(1.15 − 1,	1.16,	−1.14 − 1,	−2)
86KOR/KUK	(5.87 − 2,	0.62,	5.36 − 2,	2)	86OGA/MUR	(9.88 − 2,	1.02,	−9.88 − 2,	−1)
86TAN/TOY	(5.51 − 2,	0.56,	5.51 − 2,	1)	88AND/PAT	(1.04 − 1,	1.07,	−1.04 − 1,	−1)
88OKA/OGA	(9.04 − 2,	0.93,	−9.04 − 2,	−2)					

TABLE 3. Parameters of cubic spline polynomials for methanol

Statistics

Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C_p	113	29	1.317	3.46 − 2	1.97	5.74 − 2	1
C_{sat}	113	29	1.316	3.10 − 2	1.92	5.99 − 2	0

Parameters

Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
180.00–300.00	1.11402 + 1	−2.60664	5.13952 − 1	6.85976 − 2	I
300.00– 400.00	7.43934	1.09424	−7.19673 − 1	2.05667 − 2	III
400.00– 503.15	−5.32666 + 2	4.06173 + 2	−1.01989 + 2	8.64481	VI
180.00– 300.00	1.12658 + 1	−2.77115	5.84730 − 1	5.85928 − 2	I
300.00– 400.00	8.64423	−1.49545 − 1	−2.89140 − 1	1.55689 − 1	III
400.00– 503.15	−3.04102 + 2	2.34410 + 2	−5.89291 + 1	5.04235	VI

TABLE 4. Experimental heat capacities for ethanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method		Type capac	Calorimeter Type-Reference	
20GIB/PAR		196.2–271.4	11	nosp	not specified		C_p	IP–	20GIB/LAT
24WIL/DAN		300.0–332.0	eqn	nosp	not specified		C_p	AD–	24WIL/DAN
25PAR	N	160.0–298.0	7	0.50	not specified		C_p	IP–	25PAR
29KEL2		163.5–294.3	20	1.00	99.96	estim	C_p	IP–	29KEL1
29MIT/HAR		184.4–268.8	25	nosp	not specified		C_p	IP–	29MIT/HAR1
31BLA/LEI	N	303.1–343.1	9	3.00	not specified		C_p	IP–	31BLA/LEI
31FIO/GIN		318.1–378.1	8	0.10	not specified		C_{sat}	IP–	31FIO/GIN
36ERN/WAT		298.1	1	nosp	not specified		C_p	IP–	49WEI
39BYK		298.1	1	nosp	not specified		C_p	IP–	39BYK
49TSC/RIC2		298.1	1	nosp	not specified		C_p	IP–	49TSC/RIC1
60SWI/ZIE	N	316.5	1	nosp	not specified		C_{avg}	DR–	58SWI/ZIE1

TABLE 4. Experimental heat capacities for ethanol — Continued

Reference		Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
62RAB/NIK		288.1–328.1	9	0.30	not specified	C_p	AD– 47SKU
65KAU/BIT		293.1–349.1	11	1.0	not specified	C_p	FL– 65KAU/BIT
66HWA/ZIE		165.3–304.2	41	nosp	99.95 chrom	C_p	AD– 45SCO/MEY
66KLE		293.1–343.1	11	0.10	not specified	C_p	AD– 66KLE
67GRA		308.1–338.1	6	1.00	not specified	C_p	IP– 67GRA
67NIK/RAB		160.0–250.0	19	0.20	not specified	C_p	AD– 56POP/KOL
68PAZ/REC	N	313.1	1	nosp	not specified	C_p	CT– 70PAZ/PAZ
75PED/KAY		300.8–344.2	16	nosp	not specified	C_p	IP– 75PED/KAY
76FOR/BEN1		298.1	1	0.30	not specified	C_p	FL– 71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified	C_p	FL– 71PIC/LED
77HAI/SUG		161.3–301.1	54	nosp	99.86 melpt	C_{sat}	AD– 65SUG/SEK
78BYV/JAS		293.1–333.1	3	2.00	not specified	C_p	CT– 78BYV/JAS
79BRO/ZIE		159.0–306.0	eqn	nosp	99.94 melpt	C_p	AD– 45SCO/MEY
82BEN/DAR		288.1–308.1	2	0.30	not specified	C_p	FL– 71PIC/LED
82VIL/CAS		298.1	1	0.30	not specified	C_p	FL– 71PIC/LED
84STE/OLS		266.1–318.1	11	nosp	not specified	C_p	DS– 69PER/COM
84ZEG/SOM		298.1	1	0.30	not specified	C_p	FL– 71PIC/LED
85OGA		298.1	1	0.20	not specified	C_p	FL– 85OGA
86KOR/KUK		298.0	1	0.20	not specified	C_p	AD– 83KUK/KOR
86OGA/MUR		298.1	1	0.10	not specified	C_p	FL– 85OGA
86TAN/TOY		298.1	1	0.30	99.96 anal	C_p	FL– 71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FL– 71PIC/LED

25PAR	the same data in 27PAR/HUF
31FIO/GIN	data calculated using procedure by 85WIL/CHA
60SWI/ZIE	average value over the temperature range 294–339 K
68PAZ/REC	the same data in 70PAZ/PAZ

TABLE 5. Correlated heat capacities for ethanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$

Selected data

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
31FIO/GIN	318.1–378.1	7	0.20#	1.087	3.80–2	0.22	−1.49–2	−5
66HWA/ZIE	165.3–304.2	41	0.10#	0.440	5.73–3	0.04	1.92–3	13
66KLE	293.1–343.1	11	0.10	2.051	2.87–2	0.21	−1.29–2	−4
68PAZ/REC	313.1	1	0.30#	0.159	6.82–3	0.05	−6.82–3	−1
76FOR/BEN1	298.1	1	0.30	0.575	2.32–2	0.17	−2.32–2	−1
76FOR/BEN2	298.1	1	0.30	0.156	6.35–3	0.05	6.35–3	1
77HAI/SUG	163.1–301.1	53	0.10#	0.720	8.72–3	0.07	2.26–3	5
79BRO/ZIE	159.0–305.7	10	0.20#	0.664	1.50–2	0.13	−1.36–2	−10
86OGA/MUR	298.1	1	0.10	0.647	8.75–3	0.06	8.75	−3

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$

Rejected data

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
20GIB/PAR	(1.60–1,	1.50,	−1.32–1,	−9)	24WIL/DAN	(4.75–1,	3.01,	3.81–1,	3)
25PAR	(7.27–2,	0.55,	4.79–2,	3)	29KEL2	(8.13–2,	0.72,	−5.67–2,	−16)
29MIT/HAR	(5.35–1,	4.46,	5.15–1,	25)	31BLA/LEI	(7.79–1,	4.74,	6.94–1,	9)
36ERN/WAT	(1.08,	8.68,	−1.08,	−1)	39BYK	(5.90–2,	0.44,	−5.90–2,	−1)
49TSC/RIC2	(4.51–1,	3.23,	4.51–1,	1)	60SWI/ZIE	(1.50–1,	1.05,	−1.50–1,	−1)
62RAB/NIK	(8.45–2,	0.60,	3.37–2,	3)	65KAU/BIT	(1.50–1,	1.07,	1.34–2,	5)
67GRA	(8.73–2,	0.61,	−5.16–2,	−4)	67NIK/RAB	(6.76–2,	0.64,	−6.05–2,	−19)
75PED/KAY	(2.32–1,	1.48,	1.96–1,	14)	78BYV/JAS	(6.22–1,	4.34,	−3.37–1,	−1)
82BEN/DAR	(1.21–1,	0.87,	5.18–2,	0)	82VIL/CAS	(1.76–1,	1.29,	1.76–1,	1)
84STE/OLS	(3.98–1,	2.85,	3.90–1,	11)	84ZEG/SOM	(4.60–2,	0.34,	4.60–2,	1)
85OGA	(2.14–1,	1.61,	−2.14–1,	−1)	86KOR/KUK	(6.88–2,	0.51,	6.88–2,	1)
86TAN/TOY	(4.72–2,	0.35,	4.72–2,	1)	88AND/PAT	(9.11–2,	0.68,	−9.11–2,	−1)

TABLE 6. Parameters of cubic spline polynomials for ethanol

Statistics

Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C_p	279	126	0.892	1.51-2	0.11	-1.60-3	0
C_{sat}	279	126	0.891	1.51-2	0.11	-1.58-3	-1

Parameters

Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
159.00- 220.00	1.09275+1	9.77957-2	-7.38461-1	3.32071-1	I
220.00- 290.00	9.80965	1.62210	-1.43132	4.37050-1	I
290.00- 378.15	2.50266+1	-1.41196+1	3.99683	-1.86876-1	II
159.00- 220.00	1.08906+1	1.53924-1	-7.66644-1	3.36745-1	I
220.00- 290.00	9.86064	1.55832	-1.40500	4.33465-1	I
290.00- 378.15	2.63338+1	-1.54828+1	4.47125	-2.41965-1	II

TABLE 7. Experimental heat capacities for 1-propanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method		Type capac	Calorimeter Type-Reference	
20GIB/PAR		165.7-274.6	29	nosp	not specified		C_p	IP-	20GIB/LAT
26PAR/HUF		152.1-275.0	7	nosp	not specified		C_p	IP-	25PAR
27PAR/HUF		169.1-275.3	7	nosp	not specified		C_p	IP-	25PAR
29MIT/HAR		162.8-274.4	35	nosp	not specified		C_p	IP-	29MIT/HAR
39PHI		301.1	1	nosp	not specified		C_p	IP-	49WEI
41ZHD		279.6-318.8	5	nosp	not specified		C_p	DC-	34KOL/UDO
49TSC/RIC2		298.1	1	nosp	not specified		C_p	IP-	49TSC/RIC$_1$
51EUC/EIG		273.0-393.0	12	nosp	not specified		C_{sat}	AD-	51EUC/EIG
60SWI/ZIE	N	320.9	1	nosp	not specified		C_{avg}	DR-	58SWI/ZIE
68COU/LEE		153.9-361.5	47	0.10	99.75 melpt		C_p	AD-	63AND/COU
68PAZ/REC	N	313.1	1	nosp	not specified		C_p	CT-	70PAZ/PAZ
68REC1	N	298.0-313.0	eqn	nosp	not specified		C_p	AD-	68REC1
76FOR/BEN1		298.1-298.1	2	0.30	not specified		C_p	FL-	71PIC/LED
76FOR/BEN2		298.1	1	0.30	not specified		C_p	FL-	71PIC/LED
77MUR/SUB		298.1	1	0.30	not specified		C_p	IP-	64MOE/THO
79GRI/YAN	N	303.4-463.0	11	0.90	not specified		C_p	AD-	75RAS/GRI
80KAL/JED		181.8-303.1	66	0.20	99.95 chrom		C_p	AD-	80KAL/JED
81ARU/BAG		293.1-353.1	4	1.50	99.0 melpt		C_p	DC-	81ARU
82BEN/DAR		288.1-308.1	2	0.30	not specified		C_p	FL-	71PIC/LED
82VIL/CAS		298.1	1	0.30	not specified		C_p	FL-	71PIC/LED
84ZEG/SOM		298.1	1	0.30	not specified		C_p	FL-	71PIC/LED
86KOR/KUK		278.0-298.0	2	0.20	not specified		C_p	AD-	83KUK/KOR
86TAN/TOY		298.1	1	0.30	99.9 anal		C_p	FL-	71PIC/LED

60SWI/ZIE	average value over the temperature range 294-347 K
68PAZ/REC	the same data in 70PAZ/PAZ
68REC1	the same data in 68REC2 and 68REC3
79GRI/YAN	data above 343.3 K were measured at superambient pressures up to 1.52 MPa

TABLE 8. Correlated heat capacities for 1-propanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
51EUC/EIG	353.0–393.0	5	1.50#	0.899	3.02−1	1.35	−2.52−1	−3
68COU/LEE	153.9–361.5	47	0.10	1.227	2.18−2	0.12	2.18−3	2
76FOR/BEN1	298.1	2	0.30	0.349	1.81−2	0.10	1.64−2	2
76FOR/BEN2	298.1	1	0.30	0.021	1.08−3	0.01	1.08−3	0
79GRI/YAN	303.4–463.0	11	0.90	0.805	1.97−1	0.72	−3.58−2	−5
80KAL/JED	181.8–303.1	63	0.20	0.626	1.85−2	0.13	−5.93−3	−14
86TAN/TOY	298.1	1	0.30	0.229	1.19−2	0.07	1.19−2	1

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
					Rejected data				
20GIB/PAR	(1.03−1,	0.74,	2.14−2,	7)	26PAR/HUF	(1.26−1,	0.83,	1.17−1,	5)
27PAR/HUF	(1.21−1,	0.83,	1.16−1,	7)	29MIT/HAR	(7.89−1,	5.22,	7.30−1,	31)
39PHI	(2.30,	11.61,	2.30,	1)	41ZHD	(4.09−1,	2.17,	3.49−1,	5)
49TSC/RIC2	(5.70−1,	3.19,	5.70−1,	1)	60SWI/ZIE	(2.85−1,	1.52,	−2.85−1,	−1)
68PAZ/REC	(6.96−1,	3.65,	6.96−1,	1)	68REC1	(1.96−1,	1.10,	4.83−2,	1)
77MUR/SUB	(6.18−1,	3.45,	6.18−1,	1)	81ARU/BAG	(2.75−1,	1.39,	−2.12−1,	−2)
82BEN/DAR	(1.85−1,	1.01,	1.27−1,	0)	82VIL/CAS	(3.63−1,	2.06,	3.63−1,	1)
84ZEG/SOM	(6.96−2,	0.40,	6.96−2,	1)	86KOR/KUK	(8.74−2,	0.52,	8.65−2,	2)

TABLE 9. Parameters of cubic spline polynomials for 1-propanol

Statistics

Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C_p	241	130	0.927	9.01−2	0.38	−1.49−2	−18
C_{sat}	241	130	0.929	8.64−2	0.37	−1.45−2	−17

Parameters

Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
153.93– 260.00	9.57693	5.29059	−3.33096	8.15349−1	I
260.00– 330.00	2.47842+1	−1.22562+1	3.41780	−4.98774−2	I
330.00– 463.00	1.33110+2	−1.10734+2	3.32595+1	−3.06419	IV
153.93– 260.00	9.54635	5.33584	−3.35286	8.18814−1	I
260.00– 330.00	2.51040+1	−1.26154+1	3.55145	−6.63536−2	I
330.00– 463.00	1.37956+2	−1.15208+2	3.46402+1	−3.20663	IV

TABLE 10. Experimental heat capacities for 1-butanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
24WIL/DAN		303.0–348.0	eqn	nosp	not specified	C_p	AD– 24WIL/DAN
25PAR		194.6–294.0	12	0.50	not specified	C_p	IP– 25PAR
33TRE/WAT		298.1	1	nosp	not specified	C_p	IP– 49WEI
38PAN/DUD	N	298.0–363.0	eqn	nosp	not specified	C_p	not specified
39PHI		302.5	1	nosp	not specified	C_p	IP– 49WEI
49TSC/RIC2		298.1	1	nosp	not specified	C_p	IP– 49TSC/RIC1
60SWI/ZIE	N	322.4	1	nosp	not specified	C_{avg}	DR– 58SWI/ZIE
65COU/HAL		188.2–322.3	25	0.20	99.94 melpt	C_p	AD– 63AND/COU
67GRA		308.1–338.1	4	1.00	not specified	C_p	IP– 67GRA
68PAZ/REC	N	301.1–313.1	2	nosp	not specified	C_p	CT– 70PAZ/PAZ
75SAN	N	295.9–466.6	20	0.90	not specified	C_p	FL– 75SAN
78BYV/JAS		293.1–333.1	3	2.00	not specified	C_p	CT– 78BYV/JAS
79GRI/YAN	N	324.0–462.5	8	0.90	not specified	C_p	AD– 75RAS/GRI
81ARU/BAG		293.1–373.1	5	1.50	not specified	C_p	DC– 81ARU
86GAT/WOO		298.1–368.1	4	nosp	99. anal	C_p	DS– 83BEN/MER
86KOR/KUK		278.0–298.0	2	0.20	not specified	C_p	AD– 83KUK/KOR
86NAZ/BAS1		321.0–373.4	3	2.00	not specified	C_p	RI– 86NAZ/BAS1
86OGA/MUR		298.1	1	0.10	not specified	C_p	FL– 85OGA
86ROU/GRO		298.1	1	nosp.	99. anal	C_p	FL– 71PIC/LAD
86TAN/TOY		298.1	1	0.30	99.9 anal	C_p	FL– 71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FL– 71PIC/LED
88PIE/SOM		298.1	1	nosp	not specified	C_p	FL– 71PIC/LED

38PAN/DUD	temperature range of parameters validity estimated by the compiler
60SWI/ZIE	average value over temperature range 294–350 K
68PAZ/REC	the same data as in 70PAZ/PAZ; value at 313.15 K is apparently wrong
75SAN	isobaric heat capacities at pressure about 1.4 MPa
79GRI/YAN	data above 363.6 K were measured at superambient pressures up to 0.92 MPa

TABLE 11. Correlated heat capacities for 1-butanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	+/−
				Selected data				
65COU/HAL	188.2–322.3	25	0.20	0.830	3.48-2	0.17	3.50-3	−2
68PAZ/REC	301.1	1	0.30#	0.422	2.73-2	0.13	2.73-2	1
75SAN	295.9–466.6	19	0.90	1.078	2.79-1	0.97	−4.99-4	−2
79GRI/YAN	324.0–462.5	8	0.90	0.781	2.28-1	0.70	1.09-1	4
86GAT/WOO	298.1–368.1	4	0.30#	1.032	7.30-2	0.31	−5.26-2	−2
86OGA/MUR	298.1	1	0.10	0.095	2.03-3	0.01	2.03-3	0
86TAN/TOY	298.1	1	0.30	0.893	5.69-2	0.27	−5.69-2	−1
88AND/PAT	298.1	1	0.30#	0.571	3.65-2	0.17	−3.65-2	−1
88PIE/SOM	298.1	1	0.30#	0.156	1.00-2	0.05	−1.00-2	−1

	d/R	d_r %	d_b/R	+/−		d/R	d_r %	d_b/R	+/−
					Rejected data				
24WIL/DAN	(1.03-1,	0.43,	2.44-2,	2)	25PAR	(8.07-2,	0.40,	4.39−2,	6)
33TRE/WAT	(7.37-1,	3.34,	7.37-1,	1)	38PAN/DUD	(1.37,	5.67,	1.07,	3)
39PHI	(4.23,	16.32,	4.23,	1)	49TSC/RIC2	(8.86-1,	3.99,	8.86−1,	1)
60SWI/ZIE	(8.35-1,	3.67,	−8.35-1,	−1)	67GRA	(2.89-1,	1.23,	−2.59−1,	−4)
78BYV/JAS	(2.15,	10.11,	−1.84,	−3)	81ARU/BAG	(3.71-1,	1.50,	−3.14−1,	−3)
86KOR/KUK	(1.17-1,	0.58,	1.12-1,	2)	86NAZ/BAS1	(8.71-1,	3.31,	−8.03−1,	−3)
86ROU/GRO	(1.44-1,	0.68,	−1.44-1,	−1)					

TABLE 12. Parameters of cubic spline polynomials for 1-butanol

			Statistics				
Heat Cap. Type	No. Pnts Total	No. Pnts Used	s_w	s/R	s_r %	s_b/R	$+/-$
C_p	106	61	0.952	1.89–1	0.65	1.10–2	−4
C_{sat}	106	61	0.951	1.88–1	0.65	1.09–2	−4

		Parameters			
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
188.22– 293.00	6.76094	1.27141+1	−6.50730	1.30119	I
293.00– 363.00	1.34385+2	−1.17959+2	3.80911+1	−3.77257	III
363.00– 466.63	−1.32680+1	4.06820	4.47474	−6.85669−1	IV
188.22– 293.00	6.74763	1.27313+1	−6.51457	1.30221	I
293.00– 363.00	1.34985+2	−1.18570+2	3.82981+1	−3.79593	III
363.00– 466.63	−6.08726	−1.98117	6.18000	−8.46610−1	IV

Table 13. Experimental heat capacities for 1-pentanol

Reference		Temp. range K	No. pnts	Error %	Purity % method	Type Capac	Calorimeter Type-Reference
33PAR/HUF		204.1–298.0	6	1.00	not specified	C_p	IP– 25PAR
39PHI		302.4	1	nosp	not specified	C_p	IP– 49WEI
49LEE		313.0–343.0	eqn	nosp	not specified	C_p	CC– 33FER/MIL
49TSC/RIC2		298.1	1	nosp	not specified	C_p	IP– 49TSC/RIC1
68COU/LEE		205.1–389.1	53	0.15	99.87 melpt	C_p	AD– 63AND/COU
68PAZ/REC	N	313.1	1	nosp	not specified	C_p	CT– 70PAZ/PAZ
76SKO/SUU		298.1	1	0.10	not specified	C_p	DR– 71KON/SUU
79GRI/YAN	N	301.3–463.4	9	0.90	not specified	C_p	AD– 75RAS/GRI
81ARU/BAG		293.1–393.1	6	1.50	not specified	C_p	DC– 81ARU
83DAP/DEL		288.1–298.1	2	0.30	not specified	C_p	FL– 71PIC/LED
86BEN/DAR		298.1	1	0.30	not specified	C_p	FL– 71PIC/LED
86TAN/TOY		298.1	1	0.30	98. anal	C_p	FL– 71PIC/LED

68PAZ/REC the same data in 70PAZ/PAZ
79GRI/YAN data above 382.7 K were measured at superambient
pressures up to 0.81 MPa

TABLE 14. Correlated heat capacities for 1-pentanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
68COU/LEE	205.1–389.1	53	0.15	0.386	1.41−2	0.06	−1.97−3	−4
76SKO/SUU	298.1	1	0.10	1.229	3.08−2	0.12	3.08−2	1
79GRI/YAN	301.3–463.4	9	0.90	0.697	2.00−1	0.63	1.41−1	5
86TAN/TOY	298.1	1	0.30	0.074	5.56−3	0.02	5.56−3	1

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
				Rejected data					
33PAR/HUF	(7.74−2,	0.31,	6.67−2,	5)	39PHI	(1.18,	4.87,	−1.18,	−1)
49LEE	(1.68+1,	37.34,	1.68+1,	5)	49TSC/RIC2	(6.94−1,	2.70,	6.94−1,	1)
68PAZ/REC	(2.35,	8.12,	2.35,	1)	81ARU/BAG	(3.93−1,	1.36,	−2.93−1,	−4)
83DAP/DEL	(7.88−2,	0.32,	−7.37−2,	−2)	86BEN/DAR	(8.34−2,	0.33,	−8.34−2,	−1)

TABLE 15. Parameters of Cubic Spline Polynomials for 1-Pentanol

				Statistics				
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$	
C	87	64	0.488	8.01−2	0.25	1.88−2	3	

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
205.12– 295.00	1.17769+1	1.06001+1	−5.86915	1.27629	I
295.00– 380.00	1.62503+2	−1.42681+2	4.60905+1	−4.59485	I
380.00– 463.36	−2.84080+2	2.09885+2	−4.66900+1	3.54379	V

TABLE 16. Experimental heat capacities for 1-hexanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
29KEL2		229.6–290.0	7	1.00	not specified	C_p	IP– 29KEL1
59HUT/BAI		298.1	1	nosp	not specified	C_p	AD– 55HUT/MAN
73KAL/WOY		303.1	1	nosp	not specified	C_p	IP– 70REC
79GRI/YAN	N	303.7–462.0	9	0.90	not specified	C_p	AD– 75RAS/GRI
81ARU		293.1–393.1	6	1.50	not specified	C_p	DC– 81ARU
83BEN/DAR		298.1	1	0.30	not specified	C_p	FL– 71PIC/LED
84BRA/PIN		298.1	1	nosp	99. melpt	C_p	FL– 71PIC/LED
84KAL/WOY		229.1–300.6	35	nosp	99.9 chrom	C_p	AD– 80KAL/JED
85COS/PAT		283.1–313.1	3	0.30	98. estim	C_p	FL– 71PIC/LED
86TAN/TOY		298.1	1	0.30	98. anal	C_p	FL– 71PIC/LED
88AND/PAT		298.1	1	nosp	98. anal	C_p	FL– 71PIC/LED
89VES/BAR	N	298.1–318.1	5	0.50	not specified	C_p	AD– 79VES/ZAB

79GRI/YAN   data above 385.4 K were measured at superambient pressures up to 0.74 MPa

89VES/BAR   water content 0.04 mass per cent

TABLE 17. Correlated Heat capacities for 1-Hexanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
			Selected data					
29KEL2	229.6–290.0	7	1.00	1.344	3.41-1	1.34	−1.95-1	−5
79GRI/YAN	303.7–462.0	9	0.90	0.458	1.44-1	0.41	5.02-2	3
83BEN/DAR	298.1	1	0.30	0.298	2.58-2	0.09	2.58-2	1
84BRA/PIN	298.1	1	0.30#	1.134	9.80-2	0.34	−9.80-2	−1
84KAL/WOY	229.1–300.6	35	3.50#	0.960	9.00-1	3.36	8.93-1	35
85COS/PAT	283.1–313.1	3	0.30	1.611	1.43-1	0.48	−1.35-1	−3
86TAN/TOY	298.1	1	0.30	0.187	1.62-2	0.06	1.62-2	1
88AND/PAT	298.1	1	0.30#	1.222	1.06-1	0.37	1.06-1	1
89VES/BAR	298.1–318.1	5	0.50	1.096	1.62-1	0.55	1.27-1	4

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
				Rejected data					
59HUT/BAI	(3.19-1,	1.09,	3.19-1,	1)	73KAL/WOY	(3.66-1,	1.22,	3.66-1,	1)
81ARU	(4.94-1,	1.36,	−1.41-1,	−2)					

TABLE 18. Parameters of cubic spline polynomials for 1-hexanol

			Statistics				
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	71	63	1.055	7.20-1	2.69	4.86-1	36

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
229.14– 290.00	−5.41058+1	8.83289+1	−3.51120+1	4.97293	IV
290.00– 360.00	2.42829+2	−2.18845+2	7.08100+1	−7.20201	IV
360.00– 462.03	−1.81033+2	1.34373+2	−2.73061+1	1.88281	V

TABLE 19. Experimental heat capacities for 1-heptanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
56PAR/KEN		240.0–300.0	7	1.00	98.2 melpt	C_p	IP– 25PAR
59HUT/BAI		298.1	1	nosp	not specified	C_p	AD– 55HUT/MAN
67GRA		308.1–338.1	4	1.00	not specified	C_p	IP– 67GRA
79GRI/YAN	N	303.0–462.3	9	0.90	not specified	C_p	AD– 75RAS/GRI
80VAS/TRE		323.0–453.0	eqn	2.00	99.8 anal	C_{sat}	AD– 80VAS/TRE
88AND/PAT		298.1	1	nosp	98. anal	C_p	FL– 71PIC/LED
88NAZ/BAS		303.4–447.1	7	2.20	99.2 anal	C_p	RP– 86NAZ/BAS1
89VES/BAR	N	298.1–318.1	5	0.50	not specified	C_p	AD– 79VES/ZAB

79GRI/YAN	data above 425.2 K were measured at superambient pressures up to 0.27 MPa
89VES/BAR	water content 0.007 mass per cent

TABLE 20. Correlated heat capacities for 1-heptanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
56PAR/KEN	240.0–300.0	7	1.00	1.190	3.87–1	1.19	1.51–1	1
59HUT/BAI	298.1	1	0.50#	0.808	1.33–1	0.40	1.33–1	1
79GRI/YAN	303.0–462.3	9	0.90	0.458	1.61–1	0.41	7.75–2	5
88AND/PAT	298.1	1	0.30#	0.218	2.15–2	0.07	2.15–2	1
89VES/BAR	298.1–318.1	5	0.50	0.808	1.38–1	0.40	−1.29–1	−5

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
				Rejected data					
67GRA	(8.64–1,	2.48,	−8.56–1, −4)	80VAS/TRE	(1.00,	2.47,	−9.62–1,	−14)	
88NAZ/BAS	(1.43,	3.73,	1.83–1, 1)						

TABLE 21. Parameters of cubic spline polynomials for 1-heptanol

				Statistics				
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$	
C	48	23	0.963	2.87–1	0.85	5.51–2	3	

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
240.00– 300.00	−2.33938+2	2.82773+2	−1.03216+2	1.28701+1	IV
300.00– 360.00	4.55134+2	−4.06299+2	1.26474+2	−1.26511+1	IV
360.00– 462.31	−2.77526+2	2.04251+2	−4.31228+1	3.05233	V

TABLE 22. Experimental heat capacities for 1-octanol

Reference		Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
31CLI/AND		246.0–286.0	4	nosp	not specified	C_{sat}	DR– 26AND/LYN
59HUT/BAI		298.1	1	nosp	not specified	C_p	AD– 55HUT/MAN
61ROU		298.9–311.3	5	nosp	not specified	C_p	AD– 61ROU
79GRI/YAN		310.7–452.3	8	0.90	not specified	C_p	AD– 75RAS/GRI
80VAS/TRE		313.0–468.0	eqn	2.00	99.6 anal	C_{sat}	AD– 80VAS/TRE
86NAZ/BAS2		303.2–448.6	7	2.00	99.6 estim	C_p	RP– 86NAZ/BAS1
89VES/BAR	N	298.1–318.1	5	0.50	not specified	C_p	AD– 79VES/ZAB

89VES/BAR   water content 0.039 mass per cent

TABLE 23. Correlated heat capacities for 1-octanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
31CLI/AND	246.0–273.1	3	1.50#	0.646	3.17–1	0.97	−1.97–1	−1
61ROU	298.9–311.3	5	0.50#	1.008	1.88–1	0.50	1.50–1	3
79GRI/YAN	310.7–452.3	8	0.90	0.375	1.61–1	0.34	5.39–2	4
89VES/BAR	298.1–318.1	5	0.50	0.872	1.67–1	0.44	−1.59–1	−5

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
				Rejected data					
59HUT/BAI	(9.37−1,	2.49,	9.37−1,	1)	80VAS/TRE	(7.20−1,	1.59,	−6.59−1,	−14)
86NAZ/BAS2	(1.47,	3.36,	9.14−2,	−1)					

TABLE 24. Parameters of cubic spline polynomials for 1-octanol

				Statistics				
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	51	21	0.867	2.35–1	0.63	−9.74–3	1

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
246.00– 300.00	−7.91423+2	8.44569+2	−2.90774+2	3.37629+1	V
300.00– 360.00	4.78605+2	−4.25459+2	1.32568+2	−1.32752+1	IV
360.00– 452.29	−2.87499+2	2.12961+2	−4.47706+1	3.14507	V

TABLE 25. Experimental heat capacities for 1-nonanol

Reference	Temp. range K	No. pnts.	Error %	Purity %	method	Type capac	Calorimeter Type-Reference
79GRI/YAN	304.2–464.2	10	0.90	not specified		C_p	AD– 75RAS/GRI
82VAS/PET	303.0–423.0	eqn	nosp	99.2	anal	C_{sat}	AD– 80VAS/TRE
82VAS/PET	423.0–483.0	eqn	nosp	99.2	anal	C_{sat}	AD– 80VAS/TRE
86NAZ/BAS2	303.1–474.1	8	2.00	99.4	estim	C_p	RP– 86NAZ/BAS1

TABLE 26. Correlated Heat capacities for 1-Nonanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
79GRI/YAN	304.2–464.2	10	1.00	0.193	9.24-2	0.19	3.21-4	2

	d/R	d_r %	d_b/R	$+/-$		d/R	d_r %	d_b/R	$+/-$
				Rejected data					
82VAS/PET	(6.05−2,	1.21,	2.42−1,	2)	82VAS/PET	(8.39−1,	1.50,	8.09−1,	5)
86NAZ/BAS	(1.52,	3.02,	−8.17−1,	−2)					

TABLE 27. Parameters of cubic spline polynomials for 1-nonanol

			Statistics				
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	38	10	0.272	1.31-1	0.27	3.21-4	2

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
304.17– 380.00	2.95850+2	−2.63858+2	8.58446+1	−8.75264	IV
380.00– 464.24	−6.83055+2	5.08962+2	−1.17529+2	9.08715	IV

TABLE 28. Experimental heat capacities for 1-decanol

Reference	Temp. range K	No. pnts.	Error %	Purity %	method	Type capac	Calorimeter Type-Reference	
67GRA	308.1–338.1	4	1.00	not specified		C_p	IP–	67GRA
75WOY/KAL	303.1	1	nosp	not specified		C_p	IP–	70REC
79GRI/YAN	305.8–463.3	9	0.90	not specified		C_p	AD–	75RAS/GRI
79SVE	301.0–461.0	33	nosp	99.80	chrom	C_{sat}	DS–	69PER/COM
80VAS/TRE	323.0–403.0	eqn	2.00	99.2	anal	C_{sat}	AD–	80VAS/TRE
80VAS/TRE	403.0–503.0	eqn	2.00	99.2	anal	C_{sat}	AD–	80VAS/TRE
85COS/PAT	283.1–313.1	3	nosp	99.	estim	C_p	FL–	71PIC/LED
88AND/PAT	298.1	1	nosp	98.	anal	C_p	FL–	71PIC/LED
88NAZ/BAS	304.0–523.0	9	2.20	99.1	anal	C_p	RP–	86NAZ/BAS1

TABLE 29. Correlated heat capacities for 1–decanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
75WOY/KAL	303.1	1	0.30#	0.407	5.55–2	0.12	5.55–2	1
79GRI/YAN	305.8–463.3	9	0.90	1.251	6.45–1	1.13	4.92–1	5
79SVE	301.0–461.0	33	1.00#	0.380	2.11–1	0.38	−1.40–1	−23
80VAS/TRE	403.0–503.0	11	2.00	0.123	1.46–1	0.25	−5.01–2	−4
85COS/PAT	283.1–313.1	3	0.30#	1.027	1.41–1	0.31	−1.26–1	−3
88AND/PAT	298.1	1	0.30#	2.120	2.85–1	0.64	2.85–1	1

	d/R	d_r %	d_b/R	$+/-$			d/R	d_r %	d_b/R	$+/-$
					Rejected data					
67GRA	(1.68,	3.71,	−1.56,	−4)	80VAS/TRE		(5.97−1,	1.16,	−5.48−1,	−7)
88NAZ/BAS	(1.88,	3.15,	2.48−1,	−2)						

Table 30. Parameters of cubic spline polynomials for 1–decanol

				Statistics				
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$	
C	80	58	0.712	3.25−1	0.58	−1.37−2	−23	

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
283.15– 393.00	1.58356+2	−1.34024+2	4.65302+1	−4.82249	IV
393.00– 503.00	−4.20453+2	3.07816+2	−6.58971+1	4.71333	IV

TABLE 31. Experimental heat capacities for 1–undecanol

Reference	Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
82VAS/PET	303.0–433.0	eqn	nosp	99.7 anal	C_{sat}	AD– 80VAS/TRE
82VAS/PET	433.0–523.0	eqn	nosp	99.7 anal	C_{sat}	AD– 80VAS/TRE
87NAZ/BAD	303.6–499.6	9	nosp	not specified	C_{sat}	RP– 86NAZ/BAS1
88AND/PAT	298.1	1	nosp	98. anal	C_p	FL– 71PIC/LED

TABLE 32.   Correlated heat capacities for 1-undecanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
			Selected data					
82VAS/PET	303.0–433.0	14	2.00#	0.223	2.40−1	0.45	4.42−2	0
82VAS/PET	433.0–523.0	10	2.00#	0.136	1.79−1	0.27	1.95−2	−1
88AND/PAT	298.1	1	0.30#	0.119	1.74−2	0.04	−1.74−2	−1

	d/R	d_r %	d_b/R	$+/-$			d/R	d_r %	d_b/R	$+/-$
				Rejected data						
87NAZ/BAD	(2.92,	4.39,	1.72−3,	−3)						

Table 33.   Parameters of cubic spline polynomials for 1-undecanol

				Statistics			
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	34	25	0.211	2.37−1	0.42	3.18−2	−2

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
298.15– 420.00	−7.49134+1	6.40910+1	−8.09149	1.75215−1	V
420.00– 523.00	−2.31985+2	1.76285+2	−3.48043+1	2.29528	V

Table 34.   Experimental heat capacities for 1-dodecanol

Reference	Temp. range K	No. pnts.	Error %	Purity %	method	Type capac	Calorimeter Type-Reference	
79SVE	316.0–486.0	35	nosp	99.98	chrom	C_{sat}	DS–	69PER/COM
82VAS/PET	303.0–423.0	eqn	nosp	99.9	anal	C_{sat}	AD–	80VAS/TRE
82VAS/PET	423.0–533.0	eqn	nosp	99.9	anal	C_{sat}	AD–	80VAS/TRE
88AND/PAT	298.1	1	nosp	98.	anal	C_p	FL–	71PIC/LED

TABLE 35. Correlated heat capacities for 1–dodecanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
			Selected data					
79SVE	316.0–486.0	35	1.00#	0.163	1.04–1	0.16	−1.56–3	−7
88AND/PAT	298.1	1	0.30#	0.037	5.93–3	0.01	5.93–3	1

	d/R	d_r %	d_b/R	$+/-$			d/R	d_r %	d_b/R	$+/-$
				Rejected data						
82VAS/PET	(2.60,	4.01,	2.58,	13)		82VAS/PET	(2.60,	3.68,	2.60,	7)

TABLE 36. Parameters of cubic spline polynomials for 1–dodecanol

				Statistics			
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w %	s/R	s_r	s_b/R	$+/-$
C	61	36	0.173	1.10–1	0.17	−1.35–3	−6

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
298.15– 400.00	1.35874+2	−1.09452+2	3.99995+1	−4.24047	IV
400.00– 486.00	−5.48094+2	4.03524+2	−8.82445+1	6.44652	IV

TABLE 37. Experimental heat capacities for 1-tridecanol

Reference	Temp. range K	No. pnts.	Error %	Purity % method		Type capac	Calorimeter Type-Reference
74MOS/MOU	312.0–346.0	eqn	nosp	99.95	chrom	C_p	AD– 74MOS/MOU
80VAS/TRE	333.0–413.0	eqn	2.00	99.2	anal	C_{sat}	AD– 80VAS/TRE
80VAS/TRE	413.0–463.0	eqn	2.00	99.2	anal	C_{sat}	AD– 80VAS/TRE
80VAS/TRE	463.0–573.0	eqn	2.00	99.2	anal	C_{sat}	AD– 80VAS/TRE

TABLE 38. Correlated heat capacities for 1-tridecanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
			Selected data					
74MOS/MOU	305.0–345.0	9	0.50#	0.163	5.10–2	0.08	−9.88–3	1
80VAS/TRE	323.0–423.0	11	2.00	0.245	3.24–1	0.49	1.82–1	9
80VAS/TRE	423.0–553.0	14	2.00	0.186	2.77–1	0.37	−3.62–2	−2

TABLE 39. Parameters of cubic spline polynomials for 1-tridecanol

				Statistics			
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	34	34	0.219	2.79−1	0.40	4.14−2	8

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
305.00– 398.00	2.74994+2	−2.20393+2	7.00074+1	−6.89863	V
398.00– 553.00	−4.97352+2	3.61777+2	−7.62666+1	5.35213	V

TABLE 40. Experimental heat capacities for 1-tetradecanol

Reference	Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
74MOS/MOU	312.0–346.0	eqn	nosp	99.95 chrom	C_p	AD– 74MOS/MOU
80VAS/TRE	333.0–413.0	eqn	2.00	99.2 anal	C_{sat}	AD– 80VAS/TRE
80VAS/TRE	413.0–463.0	eqn	2.00	99.2 anal	C_{sat}	AD– 80VAS/TRE
80VAS/TRE	463.0–573.0	eqn	2.00	99.2 anal	C_{sat}	AD– 80VAS/TRE

TABLE 41. Correlated heat capacities for 1-tetradecanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
74MOS/MOU	312.0–342.0	7	0.50#	0.106	3.48−2	0.05	−8.43−3	−2
80VAS/TRE	343.0–413.0	8	2.00	0.363	5.33−1	0.73	2.89−1	4
80VAS/TRE	413.0–463.0	6	2.00	0.275	4.29−1	0.55	−1.19−1	−2
80VAS/TRE	463.0–573.0	12	2.00	0.276	4.40−1	0.55	−4.19−2	−1

TABLE 42. Parameters of cubic spline polynomials for 1-tetradecanol

				Statistics			
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	34	33	0.299	4.51−1	0.59	3.13−2	−1

			Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
312.00– 440.00	8.95398+1	−5.76851+1	2.36286+1	−2.52013	V
440.00– 573.00	−7.06941+2	4.85370+2	−9.97931+1	6.83000	V

TABLE 43. Experimental heat capacities for 1-pentadecanol

Reference	Temp. range K	No. pnts.	Error %	Purity % method		Type capac	Calorimeter Type-Reference
74MOS/MOU	318.0–346.0	eqn	nosp	99.97	chrom	C_p	AD– 74MOS/MOU
82VAS/PET	333.0–413.0	eqn	nosp	99.4	anal	C_{sat}	AD– 80VAS/TRE
82VAS/PET	413.0–513.0	eqn	nosp	99.4	anal	C_{sat}	AD– 80VAS/TRE
82VAS/PET	513.0–583.0	eqn	nosp	99.4	anal	C_{sat}	AD– 80VAS/TRE

TABLE 44. Correlated heat capacities for 1-pentadecanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
74MOS/MOU	318.0–343.0	6	0.50#	0.528	1.82–1	0.26	−7.27–2	−2
82VAS/PET	333.0–413.0	9	2.00#	0.710	1.05	1.42	1.05	9
82VAS/PET	413.0–513.0	11	2.00#	0.385	6.18–1	0.77	−3.21–1	−5
82VAS/PET	513.0–583.0	8	2.00#	0.307	5.20–1	0.61	1.99–1	4

TABLE 45. Parameters of cubic spline polynomials for 1-pentadecanol

				Statistics			
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	34	34	0.544	7.56–1	0.98	2.07–1	6

		Parameters		
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
---	---	---	---	---	---
318.00– 450.00	1.05994+2	−6.22933+1	2.31068+1	−2.33241	V
450.00– 583.00	−7.23618+2	4.90782+2	−9.97988+1	6.77171	V

TABLE 46. Experimental heat capacities for 1-hexadecanol

Reference	Temp. range K	No. pnts.	Error %	Purity % method		Type capac	Calorimeter Type-Reference
74MOS/MOU	323.0–346.0	eqn	nosp	99.96	chrom	C_p	AD– 74MOS/MOU

TABLE 47. Parameters of regression polynomial for 1-hexadecanol

		Parameters			
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
323.0– 346.0	−1.93936+1	2.76631+1			IV

TABLE 48. Experimental heat capacities for 1-octadecanol

Reference	Temp. range K	No. pnts.	Error %	Purity % method	Type capac	Calorimeter Type-Reference
80VAS/TRE	353.0–413.0	eqn	2.00	99.8 anal	C_{sat}	AD– 80VAS/TRE
80VAS/TRE	413.0–513.0	eqn	2.00	99.8 anal	C_{sat}	AD– 80VAS/TRE
80VAS/TRE	513.0–623.0	eqn	2.00	99.8 anal	C_{sat}	AD– 80VAS/TRE

TABLE 49. Correlated heat capacities for 1-octadecanol

Reference	Temp. range K	No. pnts. used	$\sigma_r C$ %	d_w	d/R	d_r %	d_b/R	$+/-$
				Selected data				
80VAS/TRE	353.0–413.0	7	2.00	0.097	1.78−1	0.19	−7.90−2	−5
80VAS/TRE	413.0–513.0	11	2.00	0.086	1.66−1	0.17	6.47−2	6
80VAS/TRE	513.0–623.0	12	2.00	0.059	1.17−1	0.12	−1.19−2	1

TABLE 50. Parameters of cubic spline polynomials for 1-octadecanol

				Statistics			
Heat Cap. Type	No. pnts. total	No. pnts. used	s_w	s/R	s_r %	s_b/R	$+/-$
C	30	30	0.087	1.66−1	0.17	5.17−4	2

		Parameters			
Temp. range K	A_0	A_1	A_2	A_3	Level of accuracy
353.00– 488.00	−4.11839+2	3.27139+2	−7.05166+1	5.09432	V
488.00– 623.00	2.67153+2	−9.02741+1	1.50188+1	−7.48262−1	V

TABLE 51. Recommended values of heat capacities

T/K	Methanol		Ethanol		1-Propanol		1-Butanol	
	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}	C_p	C_{sat}
				J K^{-1} mol^{-1}				
160			87.75	87.75	106.87	106.87		
170			88.06	88.06	107.67	107.67		
180	70.78	70.79	88.53	88.53	108.61	108.61		
190	70.78	70.79	89.17	89.17	109.72	109.72	135.95	135.95
200	70.93	70.93	90.01	90.01	111.05	111.06	137.76	137.76
210	71.24	71.23	91.05	91.05	112.65	112.65	139.80	139.80
220	71.70	71.70	92.33	92.33	114.54	114.54	142.11	142.11
230	72.32	72.32	93.84	93.84	116.77	116.77	144.76	144.76
240	73.11	73.11	95.62	95.62	119.39	119.39	147.83	147.83
250	74.06	74.06	97.68	97.68	122.43	122.43	151.38	151.38
260	75.19	75.19	100.05	100.05	125.93	125.93	155.46	155.46
270	76.49	76.49	102.74	102.74	129.92	129.92	160.15	160.15
273.15	76.93	76.93	103.67	103.67	131.29	131.29	161.77	161.77
280	77.96	77.96	105.79	105.79	134.42	134.42	165.51	165.51
290	79.62	79.62	109.21	109.21	139.42	139.42	171.61	171.61
298.15	81.11	81.10	112.29	112.29	143.86	143.86	177.16	177.16
300	81.46	81.46	113.02	113.02	144.91	144.91	178.49	178.49
310	83.50	83.48	117.22	117.21	150.90	150.90	186.06	186.06
320	85.73	85.69	121.79	121.77	157.38	157.37	194.13	194.13
330	88.17	88.11	126.73	126.68	164.34	164.33	202.51	202.51
340	90.82	90.73	132.02	131.95	171.8	171.7	211.02	211.00
350	93.71	93.57	137.66	137.54	179.5	179.5	219.46	219.43
360	96.84	96.63	143.64	143.45	187.5	187.4	227.64	227.60
370	100.22	99.93	149.95	149.68	195.4	195.3	235.4	235.3
380	103.85	103.46			203.3	203.0	242.6	242.5
390	107.76	107.24			210.9	210.4	249.3	249.1
400	112.0	111.3			218.0	217.4	255.4	255.1
410	116.5	115.6			224.5	223.7	260.9	260.5
420	121.8	120.5			230.4	229.2	265.7	265.1
430	128.2	126.1			235.3	233.7	269.8	269.0
440	136.2	132.7			239.2	237.1	273.2	272.1
450	146.2	140.6			241.9	239.3	275.8	274.3
460	158.7	150.1			243.2	240.0	277.6	275.7
470	174.0	161.3						
480	192.7	174.5						
490	215.1	190.0						
500	241.7	208.0						

T/K	1-Pentanol	1-Hexanol	1-Heptanol	1-Octanol	1-Nonanol	1-Decanol	1-Undecanol
				C			
				J K^{-1} mol^{-1}			
210	166.07						
220	168.62						
230	171.59	198.0					
240	175.05	202.7	233.7				
250	179.07	207.6	241.0	251			
260	183.70	212.8	247.2	268			
270	189.00	218.7	253.0	280			
273.15	190.83	220.7	254.8	284			
280	195.06	225.3	258.9	290			
290	201.91	233.1	265.6	298		360.8	
298.15	208.14	240.4	272.1	305.2		370.6	
300	209.64	242.2	273.8	306.9		372.9	410
310	218.14	252.2	283.8	317.5	350.1	385.5	426
320	227.21	262.9	295.4	329.5	363.7	398.5	441
330	236.60	273.9	307.7	342.5	377.7	411.4	455
340	246.09	284.8	320.3	355.6	391.5	424.2	469
350	255.45	295.2	332.4	368.2	404.7	436.5	481

TABLE 51. Recommended values of heat capacities — Continued

T/K	1-Pentanol	1-Hexanol	1-Heptanol	1-Octanol	1-Nonanol	1-Decanol	1-Undecanol
				C			
				$J\ K^{-1}\ mol^{-1}$			
360	264.46	304.9	343.5	379.7	416.9	448.2	492
370	272.87	313	353	390	427.7	458.9	502
380	280.47	321	361	398	436.6	468.5	511
390	287	327	368	405	443.3	476.6	519
400	293	333	373	410	448.2	483.1	526
410	298	338	377	414	451.7	488.1	531
420	303	342	381	417	454.2	491.8	536
430	307	346	383	420	456.2	494.4	540
440	311	349	385	421	458.1	496.1	544
450	315	351	387	423	460.4	497.2	546
460	319	354	388		463.6	498.0	548
470						498.6	549
480						499.3	550
490						500.3	550
500						501.9	551
510							551
520							551

T/K	1-Dodecanol	1-Tridecanol	1-Tetradecanol	1-Pentadecanol	1-Hexadecanol	1-Octadecanol
				C		
				$J\ K^{-1}mol^{-1}$		
300	440.8					
310	454.3	491				
320	467.9	504	535	556	574.8	
330	481.3	517	548	567	597.8	
340	494.4	530	561	579	620.8	
350	507.0	544	574	591	643.8	
360	518.8	557	586	602		745
370	529.6	570	598	613		759
380	539.3	581	609	623		770
390	547.6	591	619	633		779
400	554.3	599	628	642		786
410	559.3	605	636	651		791
420	562.8	609	643	658		795
430	565.1	612	649	665		799
440	566.5	614	653	670		801
450	567.5	615	655	674		803
460	568.2	615	656	677		804
470	569.1	615	657	678		806
480	570.4	615	657	679		807
490		615	657	680		810
500		615	657	680		813
510		615	657	681		816
520		617	657	682		820
530		620	658	685		825
540		624	662	688		830
550		630	667	694		835
560			674	701		841
570			684	711		848
580.				723		855
590						862
600						869
610						877
620						885

TABLE 52. Parameters of quasi-polynomial extrapolation equation

	Methanol	Ethanol	1-Propanol	1-Butanol	1-Pentanol
T_c/K	512.64	513.92	536.78	563.05	588.15
E_{-1}	3.88036−1	1.44763	8.39646−2	1.18513−1	2.47192
E_0	1.53705+1	2.08051+1	3.28349+1	3.07969+1	−1.97851
E_1	−1.87104+1	−3.34900+1	−1.96232+1	3.06104+1	2.05915+2
E_2	1.53026+1	2.62108+1	1.40609+1	−2.09244+1	−1.39438+2
E_3	−7.51820+1	−6.45640+1	−3.82176+2	−6.58854+2	−1.42942+3
E_4	1.84466+2	1.51592+2	8.21541+2	1.35112+3	2.90385+3
E_5	−1.20695+2	−9.49146+1	−4.70937+2	−7.38872+2	−1.57311+3
s/R	1.48	2.46−2	1.30−1	3.42−1	1.70−1
Level of accuracy	V	II	IV	V	IV

	1-Hexanol	1-Heptanol	1-Octanol	1-Nonanol	1-Decanol
T_c/K	610.70	632.50	652.50	671.50	689.00
E_{-1}	1.34814+1	9.63250+1	5.07580+1	3.85829+1	3.72491+1
E_0	−1.28058+2	−9.51594+2	−4.64298+2	−3.19775+2	−3.04549+2
E_1	6.79675+2	3.35914+3	1.67352+3	1.15290+3	1.13039+3
E_2	−4.51822+2	−2.21545+3	−9.84434+2	−5.88093+2	−5.93279+2
E_3	−2.85553+3	−9.76192+3	−4.59810+3	−2.87080+3	−2.85866+3
E_4	5.69473+3	1.93148+4	8.11435+3	4.39320+3	4.50104+3
E_5	−3.02851+3	−1.01910+4	−3.81855+3	−1.79278+3	−1.88987+3
s/R	4.68−1	3.02−1	3.76−1	3.26−1	3.65−1
Level of accuracy	V	IV	V	IV	IV

6. Figures
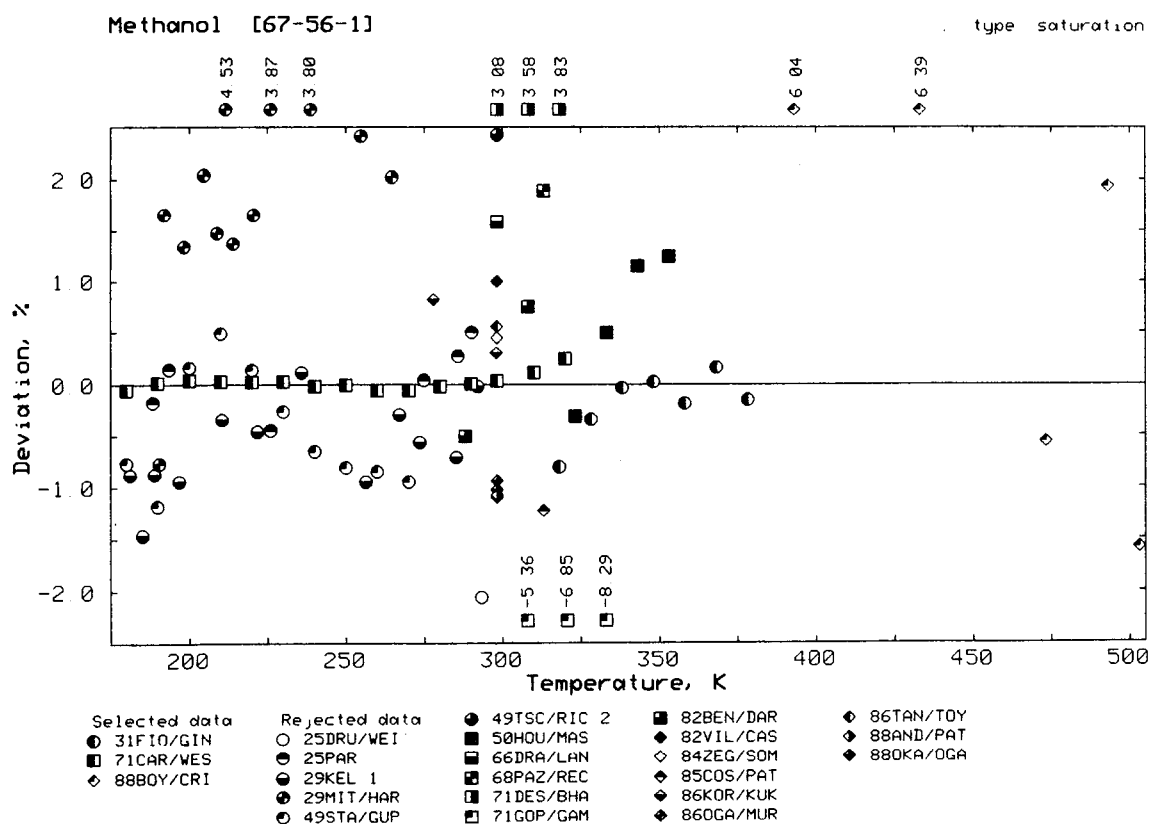
FIG. 1. Deviation plot for methanol

Ethanol [64-17-5]   type saturation

FIG. 2. Deviation plot for ethanol

1-Propanol [71-23-8]   type saturation

FIG. 3. Deviation plot for ethanol

1-Butanol [71-36-3]   type saturation
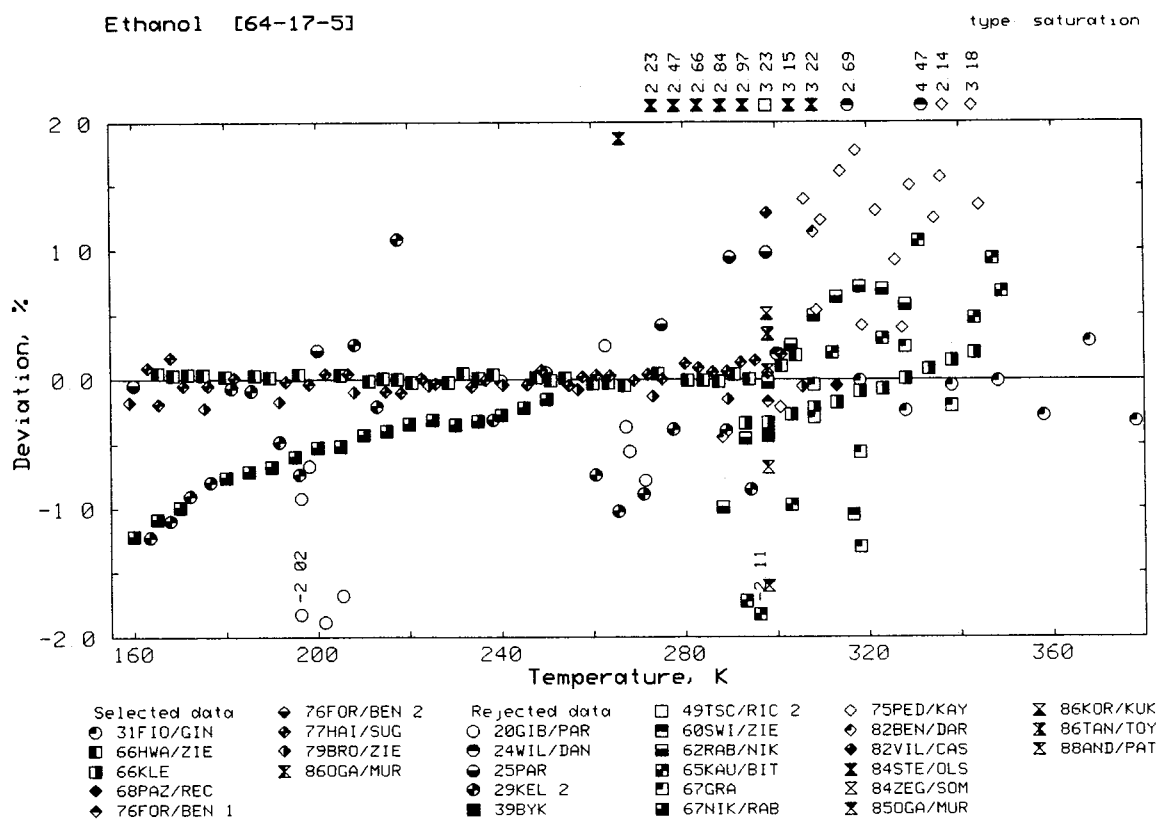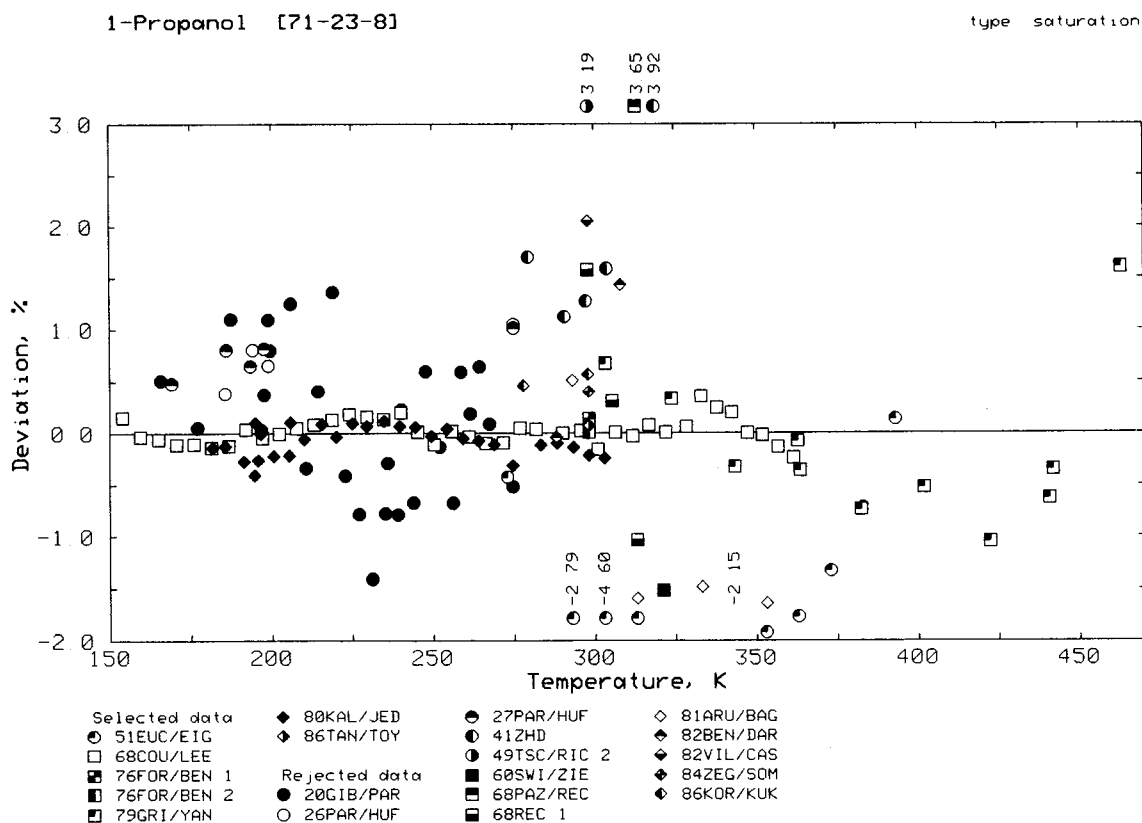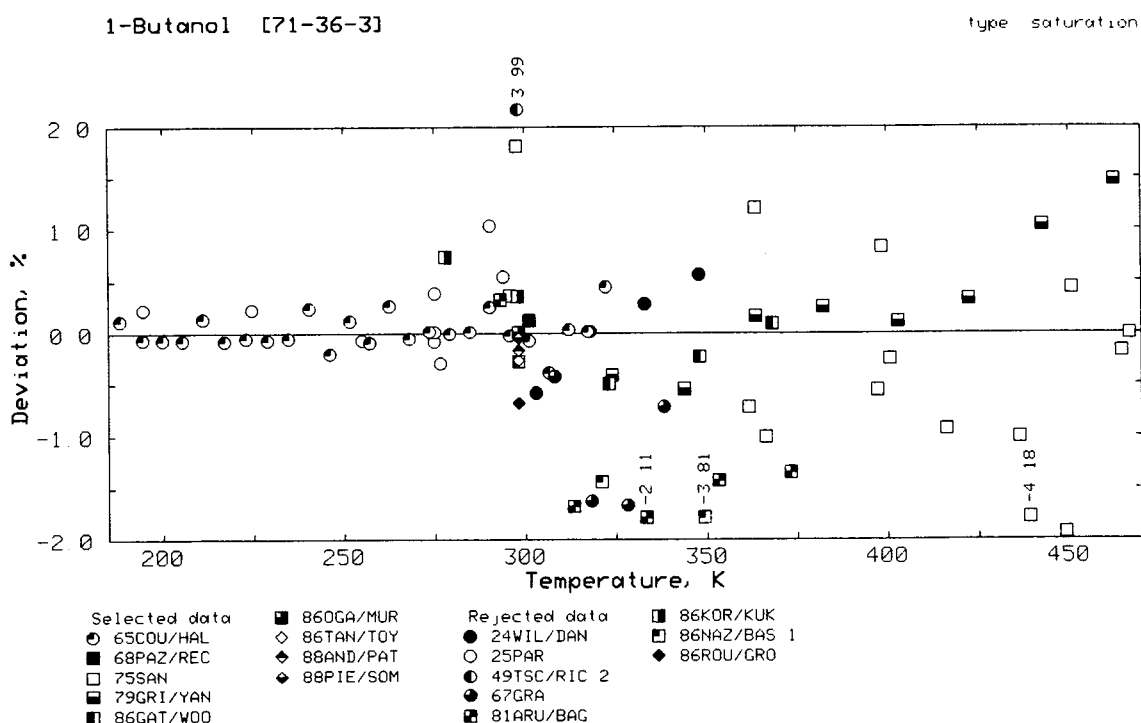
FIG. 4. Deviation plot for 1-butanol

1-Pentanol [71-41-0]
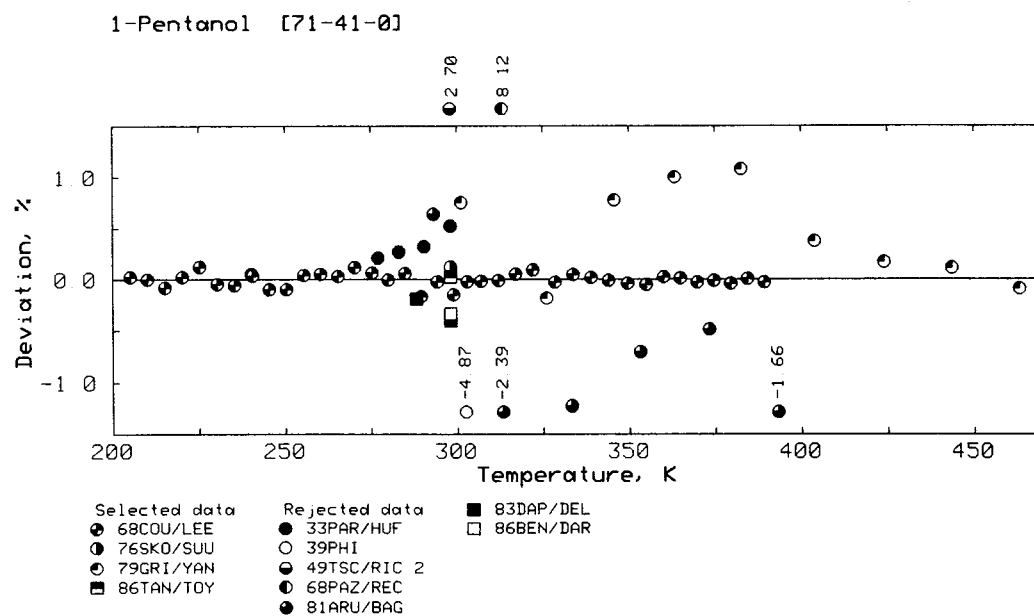
FIG. 5. Deviation plot for 1-pentanol

1-Hexanol   [111-27-3]
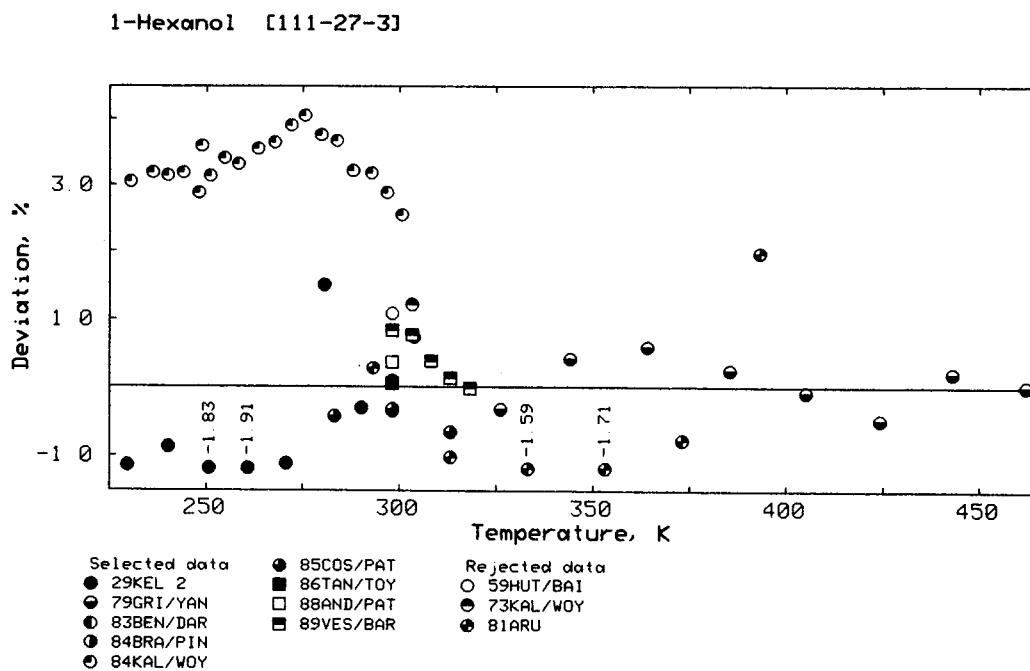
FIG. 6. Deviation plot for 1-hexanol

1-Heptanol   [111-70-6]
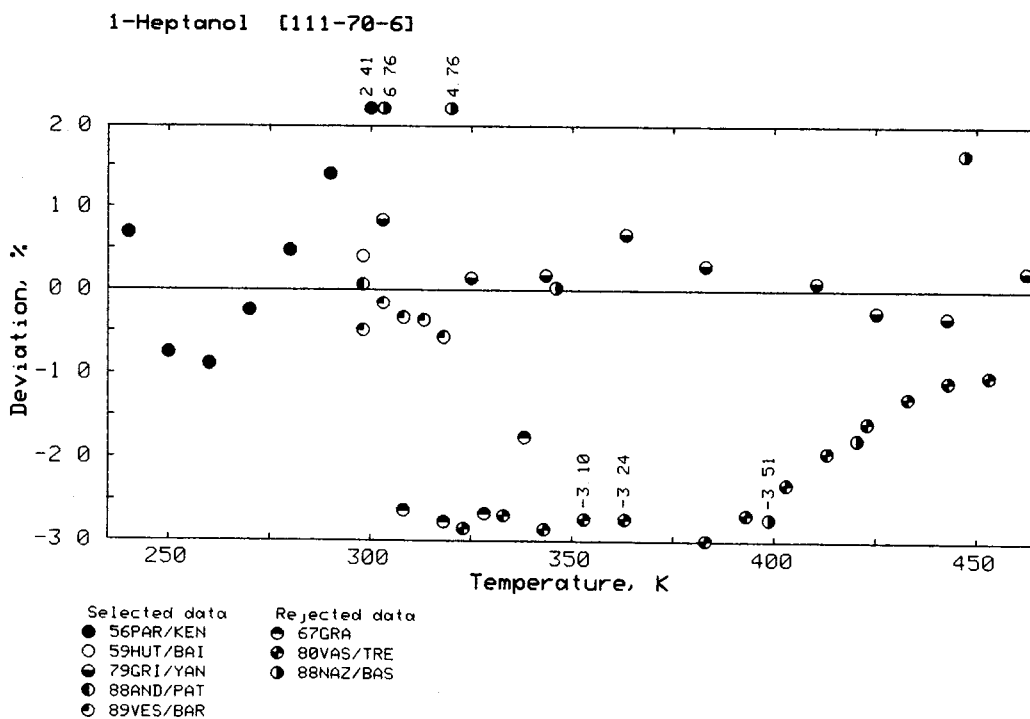
FIG. 7. Deviation plot for 1-heptanol
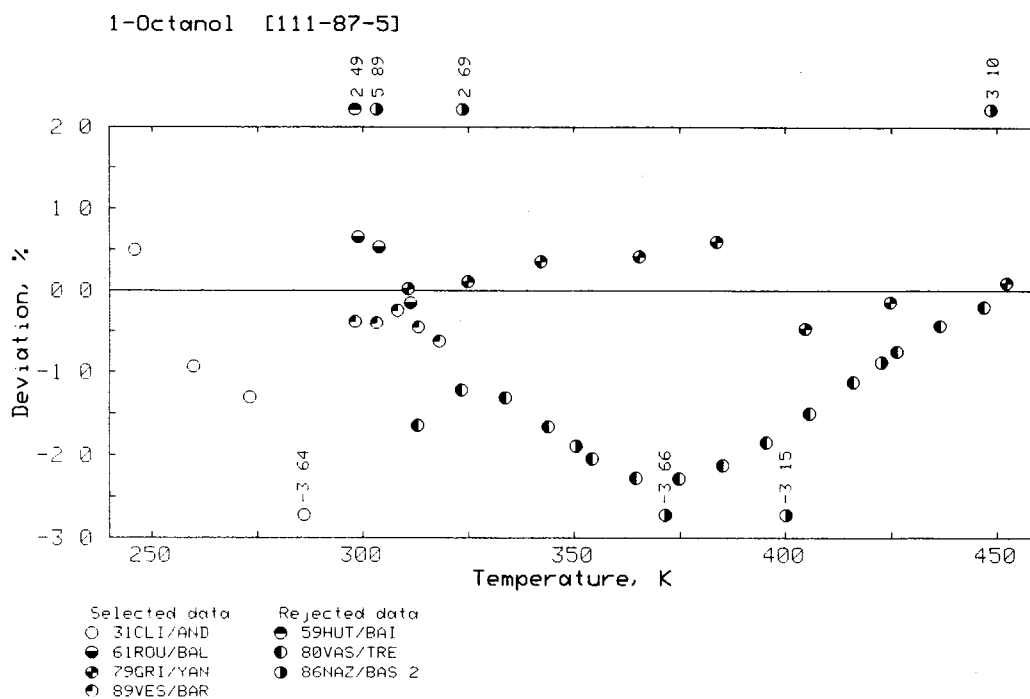
1-Octanol   [111-87-5]

FIG. 8. Deviation plot for 1-octanol

1-Nonanol   [143-08-8]
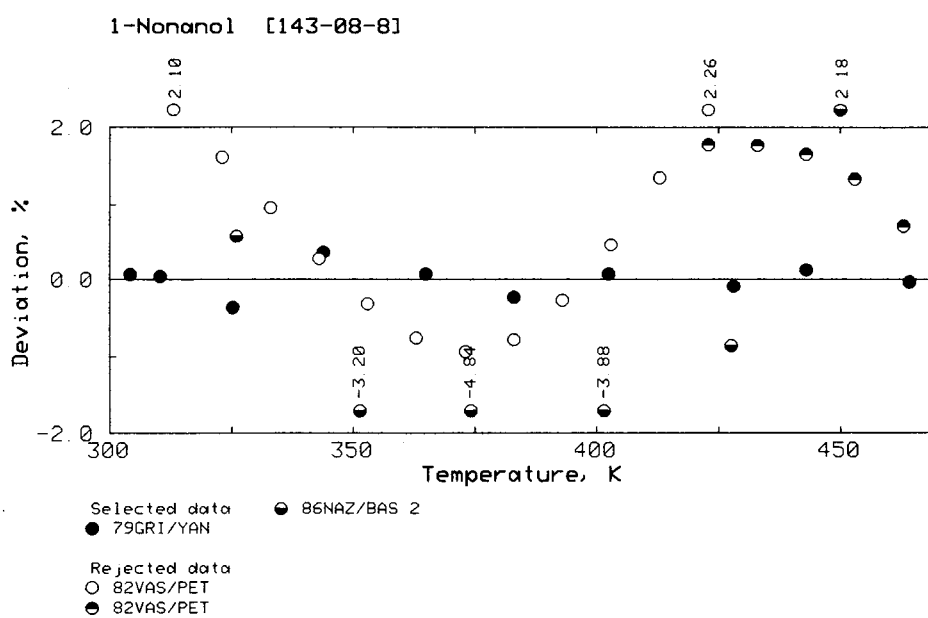
FIG. 9. Deviation plot for 1-nonanol
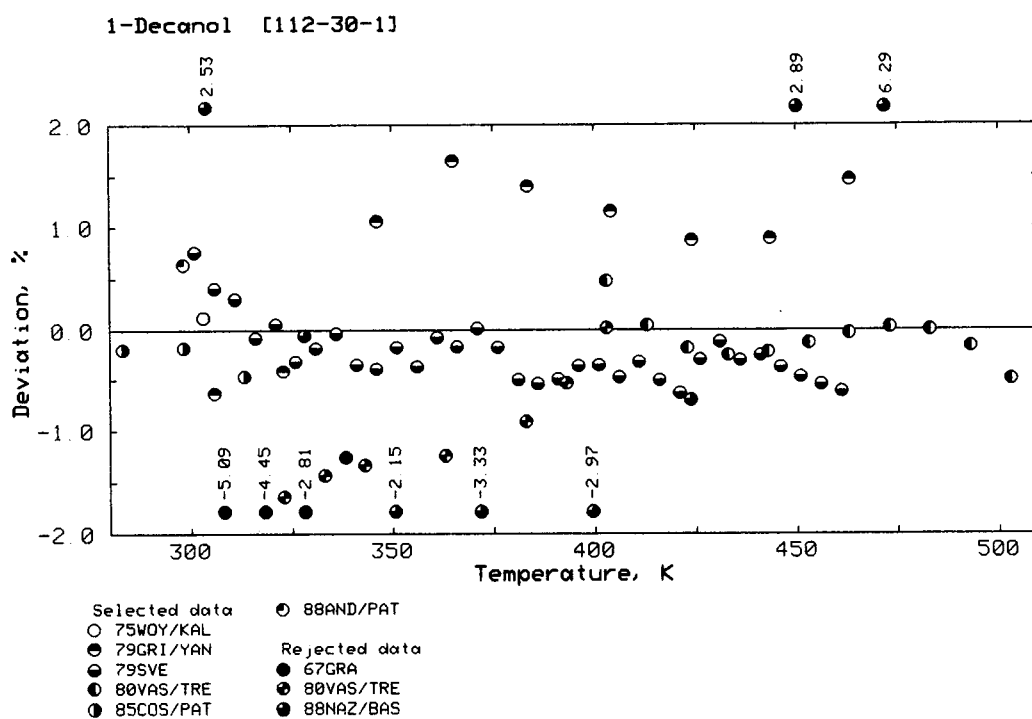
1-Decanol　[112-30-1]

FIG. 10. Deviation plot for 1-decanol
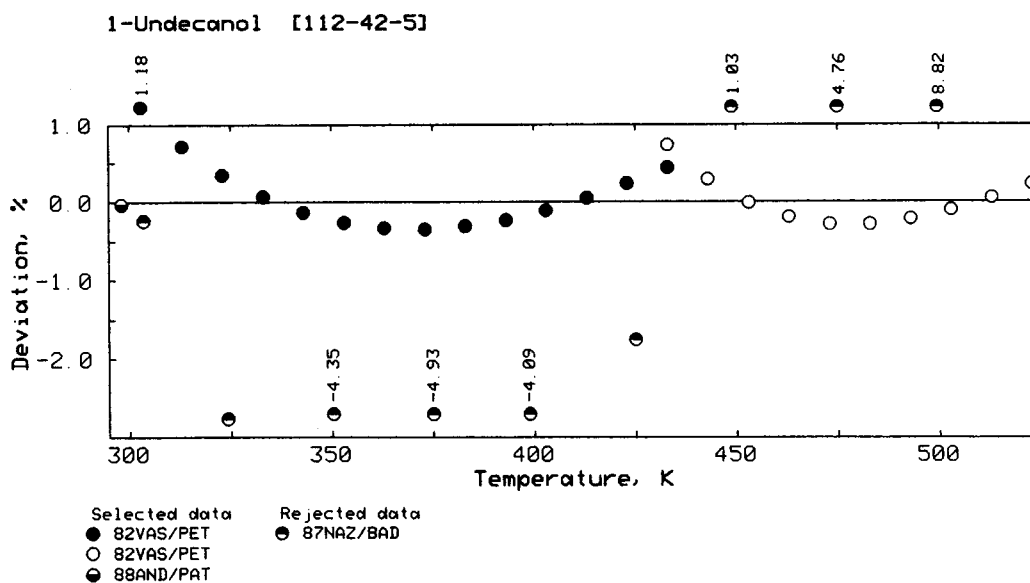
1-Undecanol　[112-42-5]

FIG. 11. Deviation plot for 1-undecanol
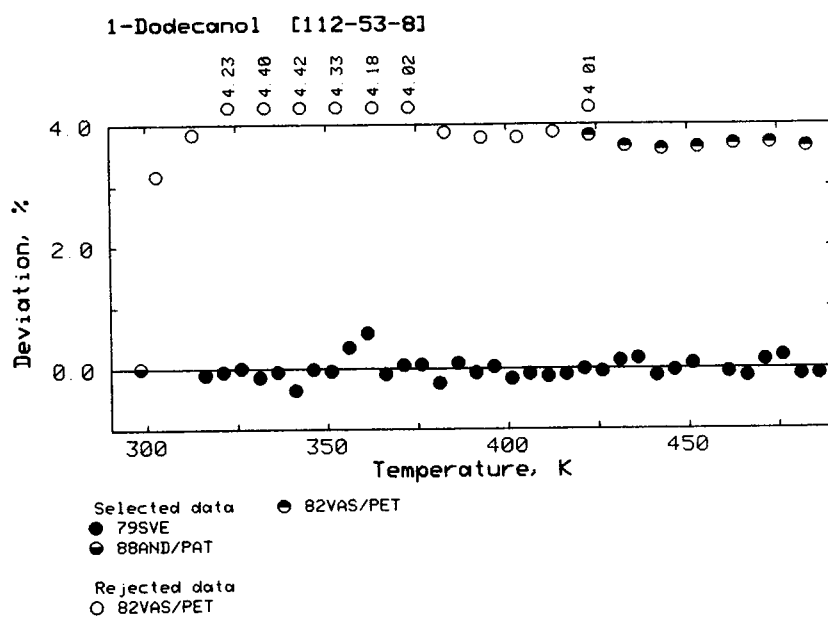
FIG. 12. Deviation plot for 1-dodecanol
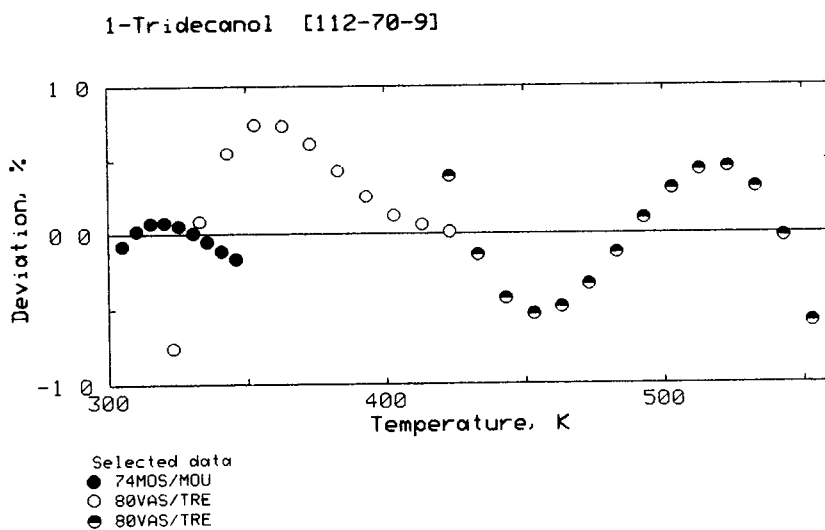
FIG. 13. Deviation plot for 1-tridecanol

1-Tetradecanol   [112-72-1]
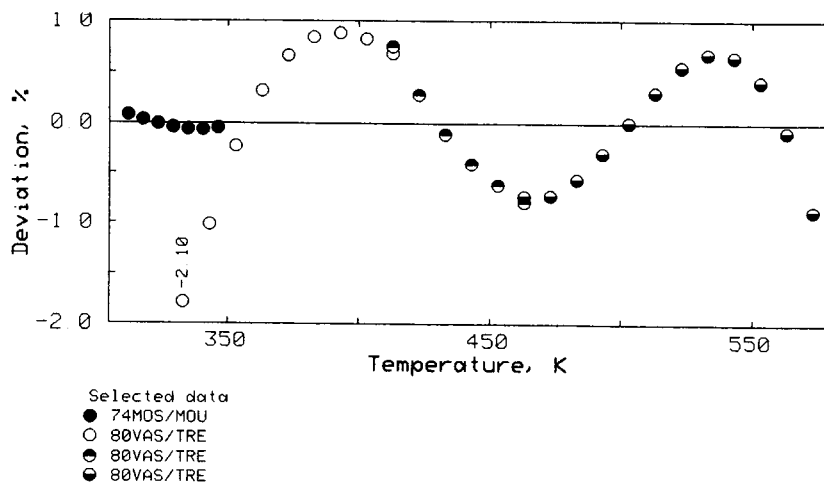
FIG. 14. Deviation plot for 1-tetradecanol

1-Pentadecanol   [629-76-5]
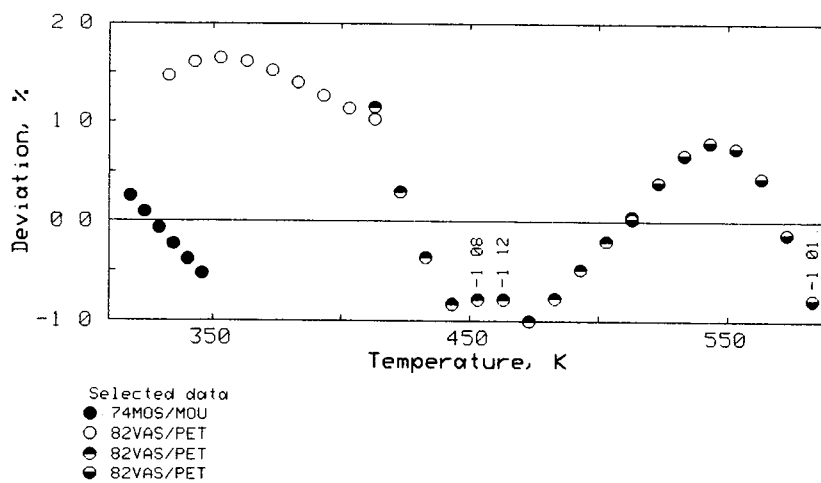
FIG. 15. Deviation plot for 1-pentadecanol

1-Octadecanol [112-92-5]
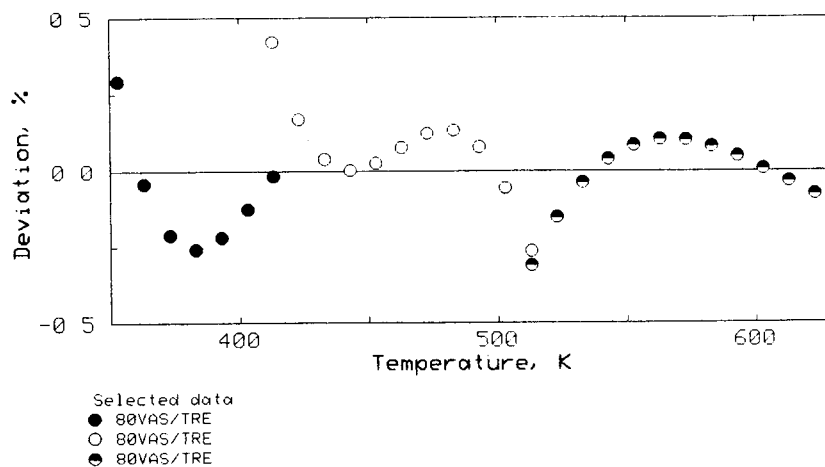
FIG. 16. Deviation plot for 1-octadecanol
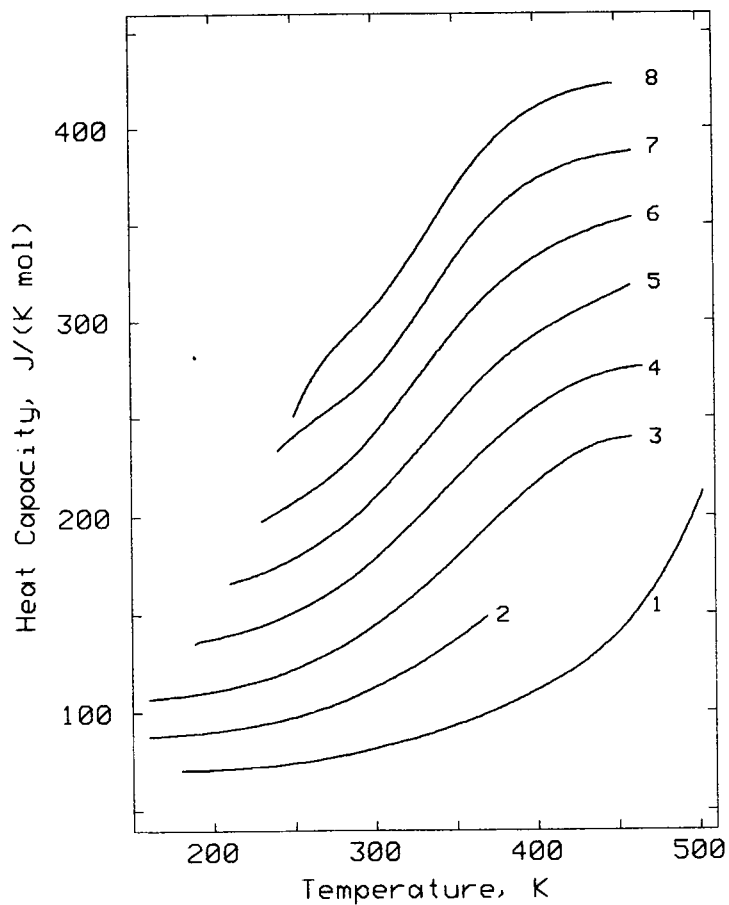
FIG. 17. Temperature dependence of saturation
heat capacity for C_1 to C_8 1-alkanols
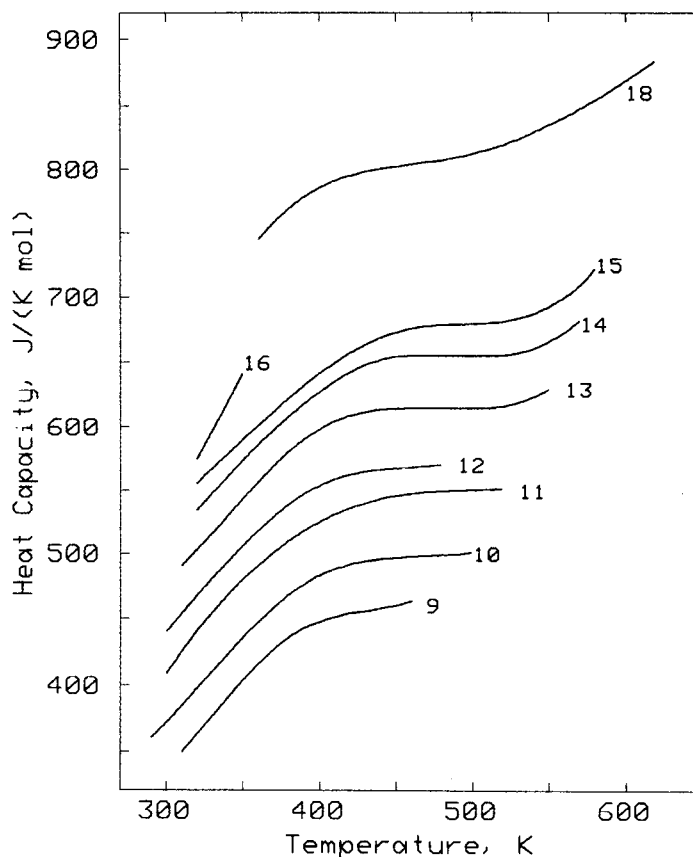
FIG. 18. Temperature dependence of saturation
heat capacity for C_9 to C_{18} 1-alkanols

7. Acknowledgement

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