Simultaneous Treatment of Vapor Pressures and Related Thermal Data Between the Triple and Normal Boiling Temperatures for *n*-Alkanes C_5 – C_{20}

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Experimental vapor pressures, calorimetric enthalpies of vaporization and differences between the heat capacities of the ideal gas and the liquid for *n*-alkanes C_5 to C_{20} between the triple and normal boiling temperatures have been treated simultaneously. Attention was focused particularly on the region of low pressures where vapor pressure data are scarce and subject to important systematic errors. The reliability and consistency of data from different sources was evaluated and the three parameter Cox equation was used to correlate simultaneously as a function of temperature the selected values of different properties. The recommended vapor pressures and thermal data resulting from this procedure are mutually consistent over the homologous series and present a considerable refinement particularly at lower pressures.

Key words: *n*-alkanes, Cox equation, critical review of data, enthalpy of vaporization, heat capacity, temperature correlation, vapor pressure.

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1. Introduction

The vapor-liquid saturation line in a diagram of pressure versus temperature is the main characteristic of the vaporization equilibrium for a one component system. The vapor pressure p_{sat} is one of the most frequently measured thermodynamic properties for pure organic liquids, and the normal boiling temperature T_b is a basic physicochemical parameter for any substance. The experimental determination of vapor pressure is relatively easy in the range between 1 and 200 kPa which is usually denoted as a moderate (or medium) pressure range (80AMB/DAV, 85AMB). Most published data have been reported between 5 and 100 kPa and many reliable results are available. The best accuracy can be achieved near the normal boiling temperature: the high quality data measured close to atmospheric pressure have an error below 0.01 percent. Measurements become difficult at low pressures (say $p_{sat} < 1$ kPa); data are available only for a limited number of substances and subject to large systematic errors. Differences in reported values usually amount to several tens of percent near the triple point temperature.

Thermal data relating to the vaporization equilibria of most interest are enthalpy of vaporization ΔH_{vap} and the difference between the heat capacity of saturated vapor C_p^g and that of the saturated liquid C_p^l

$$\Delta C_{vap} = C_p^g - C_p^l . \quad (1)$$

This quantity has a close relation to the difference between the heat capacity of ideal gas C_p° and that of the saturated liquid

$$\Delta C^{\circ}_{vap} = C_p^{\circ} - C_p^{l} \quad (2)$$

(denoted subsequently as simply the heat capacity difference) which can be easily calculated for many compounds from literature data. At pressures below 10 kPa the difference between ΔC_{vap} and ΔC°_{vap} is comparable with or lower than the experimental uncertainty and both quantities become exactly identical at the zero pressure limit.

Unlike vapor pressures, thermal properties are known for a considerable number of organic compounds with reasonable accuracy at pressures well below the normal boiling temperature. Enthalpies of vaporization have

been reported for several hundred organic compounds at or near 298.15 K which is well below T_b for many organic compounds. Heat capacities of the ideal gas, calculated from spectral data, are available for a large number of compounds at temperatures below T_b and heat capacities of liquids are accessible from calorimetric measurements down to the triple point.

Vapor pressure, enthalpy of vaporization and ΔC°_{vap} are related by exact thermodynamic relationships allowing the simultaneous correlation of experimental data as a function of temperature with a single equation. Such a treatment can serve as an efficient consistency test in data evaluation. Furthermore, the simultaneous correlation of several properties available over different temperature ranges allows an extrapolation controlled by the exact thermodynamic constraints; this can be considered as the main advantage of the procedure. In this way reliable experimental p_{sat} data in the moderate pressure range can be easily extrapolated with the support of the corresponding thermal data down to the triple point temperature. The same approach can also serve to calculate new or to refine present enthalpies of vaporization at conditions far below the normal boiling temperature by combining vapor pressures with heat capacity data. This is particularly interesting for calculating ΔH_{vap} for high boiling point compounds at 298.15 K where this property is frequently requested and not usually available with sufficient accuracy.

Volumetric properties of the saturated equilibrium phases appear in the relationships linking vapor pressures and related thermal data. These properties have little effect in the case of a saturated liquid; however, accurate determination of the molar volume and its derivatives for the saturated vapor becomes important as the vapor pressure increases and deviations from ideal-gas behavior become significant. The simultaneous treatment of vapor pressures and the thermal data is therefore suitable only at conditions below the normal boiling temperature because a risk of distortion due to the errors in the expression of vapor nonideality makes this approach ineffective at higher temperatures.

The described procedure was first used by King and Al-Najjar (74KIN/ALN) to obtain reliable values in the low pressure range for eight *n*-alkanes C_6 to C_{16} and later by Ambrose and Davies (80AMB/DAV) and Růžička and Majer (86RUZ/MAJ) for polar compounds. Several attempts were made to develop a predictive scheme based on this approach (85ROG, 86GUT, 86KIN/MAH, 88VET, 91VET); the thermodynamic basis and merits of this technique has been discussed by several authors (82MOS/VUG, 85AMB, 88MAJ/RUZ, 89LIC, 89MAJ/SVO).

Liquid *n*-alkanes and 1-alkanols are basic organic chemicals for which the thermodynamic properties are frequently demanded both in science and technology. Most thermodynamic databases such as TRC tables, DIPPR, PPDS or DECHEMA contain recommendations for these two classes of compounds which differ more or less from each other. In order to upgrade the existing recommendations and to supply verified information on phase equilibria the Subcommittee on Thermodynamic Data of the IUPAC Commission on Chemical Thermodynamics initiated a data project on "The Vapor-Liquid Equilibria in 1-Alkanol + *n*-Alkane Mixtures". Besides reports on mixture properties, several review articles have been published presenting recommended data for the thermodynamic properties of pure substances at the conditions of saturation. Recommendations for vapor pressures and critical properties were published by Ambrose and Walton (89AMB/WAL), calorimetric data on enthalpies of vaporization were compiled and the recommended values produced by Majer and Svoboda (85MAJ/SVO); the heat capacities for liquids were evaluated by Zábranský and coworkers (90ZAB/RUZ, 91RUZ/ZAB), the second virial coefficients by Dymond and coworkers (86DYM, 89TSO/DYM) and the densities of saturated liquids by Cibulka (93CIB).

Regarding vaporization equilibria most previous reports focused attention primarily on the medium and (to some extent) the high pressure ranges. Little attention was given to low pressures. In our investigation we have compiled all available p_{sat} values in the low pressure range and treated them in the region between T_t and T_b simultaneously with the other experimental data recommended in the above articles and additional recent sources. The purpose of our effort was mainly to:

a. assess all available p_{sat} data in the low pressure region;

b. examine the consistency of experimental vapor pressures with the enthalpies of vaporization and heat capacity differences between T_t and T_b;

c. produce recommended values of vapor pressures and enthalpies of vaporization in the low pressure region which would smoothly join the recent recommendations for the region of medium pressures.

In this contribution we report the results for C_5 to C_{20} *n*-alkanes. A similar treatment for 1-alkanols will be published subsequently in this Journal.

2. Thermodynamic Background

2.1. Basic Relationships

Vapor pressure p_{sat} and enthalpy of vaporization ΔH_{vap} are related by the Clapeyron equation:

$$RT^2\left(\frac{d\ln p}{dT}\right)_{sat} = \frac{\Delta H_{vap}}{\Delta Z_{vap}} \tag{3}$$

where subscript s denotes a derivative along the saturation line and $\Delta Z_{vap} = Z^g_{sat} - Z^l_{sat}$ stands for the difference between the compressibility factors of the saturated vapor and the saturated liquid. The symbol $\Delta H'$ will be used below to denote the ratio of enthalpy of vaporization and the difference in the compressibility factors

$$\Delta H' = \frac{\Delta H_{vap}}{\Delta Z_{vap}}. \tag{4}$$

For convenience let us define a new quantity $\Delta C'$ as temperature derivative of $\Delta H'$ along the saturation line

$$\Delta C' = \left(\frac{\mathrm{d}\,\Delta H'}{\mathrm{d}T}\right)_{\mathrm{sat}}. \tag{5}$$

By combining Eqs. (4) and (5) one obtains

$$\Delta C' = \left(\frac{\mathrm{d}\Delta H_{\mathrm{vap}}}{\mathrm{d}T}\right)_{\mathrm{sat}} \frac{1}{\Delta Z_{\mathrm{vap}}} - \left(\frac{\mathrm{d}\Delta Z_{\mathrm{vap}}}{\mathrm{d}T}\right)_{\mathrm{sat}} \frac{\Delta H_{\mathrm{vap}}}{\Delta Z_{\mathrm{vap}}^2}. \tag{6}$$

This relationship can be further rewritten as

$$\Delta C' = \frac{\Delta C_{\mathrm{vap}} - 2\,\Delta H'\left(\frac{\partial\,\Delta Z_{\mathrm{vap}}}{\partial T}\right)_p - \frac{p_{\mathrm{sat}}}{RT^2}\,\Delta H'^2\left(\frac{\partial\,\Delta Z_{\mathrm{vap}}}{\partial p}\right)_T}{\Delta Z_{\mathrm{vap}}} \tag{7}$$

where the difference in the heat capacities of the saturated phases ΔC_{vap} was defined by Eq. (1). The heat capacity of the saturated gas is connected with the heat capacity of an ideal gas C°_{vap} by the well known relationship

$$C_p^{\mathrm{g}} = C_p^{\circ} - T\int_0^{p_{\mathrm{sat}}} \left(\frac{\partial^2 V^{\mathrm{g}}}{\partial T^2}\right)_p \mathrm{d}p \tag{8}$$

which allows us to relate $\Delta C^{\circ}_{\mathrm{vap}}$ (see Eq. 2) directly to $\Delta C'$. The volumetric properties of the vapor phase at conditions below the normal boiling temperature can be most suitably described by the volume-explicit virial expansion truncated after the second virial coefficient B

$$V^{\mathrm{g}} = \frac{RT}{p_{\mathrm{sat}}} + B. \tag{9}$$

The difference in the compressibility factors of the saturated phases can be then written as

$$\Delta Z_{\mathrm{vap}} = 1 + \frac{p_{\mathrm{sat}}}{RT}(B - V^{\mathrm{l}}) \tag{10}$$

where the coefficient B is a function of temperature. By combining Eqs. (3), (4) and (10) one obtains

$$\Delta H' = \frac{\Delta H_{\mathrm{vap}}}{1 + \frac{p_{\mathrm{sat}}}{RT}(\mathrm{B} - V^{\mathrm{l}})}, \tag{11}$$

and similarly by combining Eqs. (7), (8) and (10) the relationship between $\Delta C'$ and the heat capacity difference $\Delta C^{\circ}_{\mathrm{vap}}$ results in the following relationship

$$\Delta C' = \Delta C^{\circ}_{\mathrm{vap}} - Tp_{\mathrm{sat}}\frac{\mathrm{d}^2 B}{\mathrm{d}T^2} - 2T\frac{\mathrm{d}(B - V^{\mathrm{l}})}{\mathrm{d}T}\left(\frac{\mathrm{d}p}{\mathrm{d}T}\right)_{\mathrm{sat}} - T(\mathrm{B} - V^{\mathrm{l}})\left(\frac{\mathrm{d}^2 p}{\mathrm{d}\,T^2}\right)_{\mathrm{sat}}. \tag{12}$$

where the pressure dependence of V^{l} was neglected. Equations (11) and (12) allow conversion of the experimentally accessible quantities ΔH_{vap} and $\Delta C^{\circ}_{\mathrm{vap}}$ to $\Delta H'$ and $\Delta C'$. For calculating the volumetric terms on the right-hand side of Eqs. (11) and (12), only the second virial coefficient and vapor pressure as a function of temperature are needed. The molar volume of the saturated liquid and its derivatives play only a minor role below the normal boiling temperature and even a rough estimation is satisfactory. At low p_{sat} the behavior of the saturated vapor is close to that of the ideal gas and ΔH_{vap}, $\Delta C^{\circ}_{\mathrm{vap}}$ are practically equal to $\Delta H'$, $\Delta C'$, respectively. The importance of the correction for the vapor nonideality increases rapidly, however, with increasing vapor pressure. This is documented in the Table 1 where the overall effect of the volumetric correction terms at different pressures is illustrated for heptane. While the enthalpy of vaporization is only moderately affected, the magnitude of the heat capacity difference and the corresponding volumetric term in Eq. (12) become comparable near atmospheric pressure; proper attention must therefore be paid to this circumstance during calculations. The growth of the difference between $\Delta C'$ and $\Delta C^{\circ}_{\mathrm{vap}}$ with increasing vapor pressure p_{sat} is also apparent from Fig. 1.

By combining Eqs. (3) and (4) we get

$$\Delta H' = RT^2\left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)_{\mathrm{sat}} = -R\left(\frac{\mathrm{d}\ln p}{\mathrm{d}(1/T)}\right)_{\mathrm{sat}}, \tag{13}$$

and by introducing this relationship into Eq. (5) it follows

$$\Delta C' = R\left[\frac{\mathrm{d}}{\mathrm{d}T}T^2\left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)\right]_{\mathrm{sat}} = 2RT\left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)_{\mathrm{sat}} + RT^2\left(\frac{\mathrm{d}^2\ln p}{\mathrm{d}T^2}\right)_{\mathrm{sat}}. \tag{14}$$

The last two relationships allow the expression of $\Delta H'$ and $\Delta C'$ exclusively from a vapor pressure equation. This means that after selecting a suitable relationship describing p_{sat} versus T it is possible to correlate simultaneously experimental p_{sat}, ΔH_{vap} and $\Delta C^{\circ}_{\mathrm{vap}}$ as a tion of temperature. The parameters of a vapor pressure equation can be obtained by minimizing an objective tion S which can be defined as

$$S = \sum_{i=1}^{I}\frac{\left(\ln p_{\mathrm{sat}}^{\mathrm{exp}} - \ln p_{\mathrm{sat}}^{\mathrm{sm}}\right)_i^2}{\sigma_i^2 \ln p_{\mathrm{sat}}} + K_H^2\sum_{j=1}^{u}\frac{\left(\Delta H'^{\mathrm{exp}} - \Delta H'^{\mathrm{sm}}\right)_j^2}{\sigma_j^2 \Delta H'} + K_C^2\sum_{k=1}^{v}\frac{\left(\Delta C'^{\mathrm{exp}} - \Delta C'^{\mathrm{sm}}\right)_k^2}{\sigma_k^2 \Delta C'}. \tag{15}$$

The quantities with the superscript "exp" relate to the experimental data ($\Delta H'^{\mathrm{exp}}$ and $\Delta C'^{\mathrm{exp}}$ are calculated from thermal data using Eqs. (11) and (12)); the quantities

with the superscript "sm" are expressed from a vapor pressure equation ($\Delta H'^{sm}$ and $\Delta C'^{sm}$ are calculated from Eqs. (13) and (14)). Indices t, u, v indicate the total number of p_{sat}, ΔH_{vap} and ΔC°_{vap} values, respectively. The variances $\sigma^2 \ln p_{sat}$, $\sigma^2 \Delta H'$ and $\sigma^2 \Delta C'$ were estimated from the expected errors of experimental data points (see Sec. 3.3.) and K_H, K_C are the weighting factors of the thermal properties in determining the parameters of a vapor pressure equation.

2.2. Vapor Pressure Equations

Selection of a flexible relationship, which enables the simultaneous description of several thermodynamic properties as a function of temperature, is crucial for the success of this correlation. We have tested extensively the performance of different correlation equations. The results of this analysis will be reported in detail elsewhere (94RUZ/MAJ), so only the main conclusions are reviewed here.

In the past relationships of the type

$$\ln p_{sat} = \sum_{i=k}^{m} A_i \times T^{i-1} + A_{\ln} \ln T \qquad (16)$$

were used in simultaneous correlation (74KIN/ALN, 80AMB/DAV, 86RUZ/MAJ) with i changing most often from 0 to 2 or 3. In this case the temperature dependence of $\Delta C'$ is expressed from Eq. (14) simply as a first or second degree polynomial which compares reasonably well with the actual shape of the $\Delta C'$ versus T curve (see Fig. 1). This is, however, the only observation in favor of these classical equations; their parameters tend to be ill-conditioned when used in the correlation of vapor pressures alone (89MAJ/SVO). When comparing expressions, the performance of Eq. (16) in the simultaneous correlation is generally worse compared to other relationships with the same number of parameters as discussed below.

In examining the correlation equations we have focused our attention especially on the Wagner equation

$$\ln\left(\frac{p_{sat}}{p_o}\right) = \frac{T_c}{T} \sum_{i=1}^{m} A_i \left(1 - \frac{T}{T_c}\right)^{\alpha_i} \qquad (17)$$

(c denotes the critical quantities) with m equal to 4 and the most common values of α_i (1,1.5,2.5,5) and to the Cox equation

$$\ln\left(\frac{p_{sat}}{p_o}\right) = \left(1 - \frac{T_o}{T}\right) \exp\left(\sum_{i=0}^{m} A_i T^i\right) \qquad (18)$$

where T_o and p_o denote an arbitrary reference temperature and the corresponding vapor pressure, respectively, m is equal to 2 or 3. Relationships (17) and (18) have been used frequently in literature for correlating p_{sat} data over a wide temperature range. The Wagner equation has recently become the standard relationship for the description of vapor pressure data up to the critical point.

In testing the performance of equations in the simultaneous correlation, the best results were achieved always with the four-parameter Cox equation using the normal boiling conditions as a reference, although for n-alkanes signs of overfitting were observed (large standard deviations in parameters). The three-parameter Cox equation and the Wagner equation performed similarly in the case of n-alkanes, where satisfactory description was obtained with both equations. The Wagner equation was, however, clearly inferior to the Cox equations when fitting the data for 1-alkanols. Although we were tempted to use the Wagner equation because of its large use and popularity in recent years, we have finally opted in this contribution for the three-parameter Cox equation. The reasons were as follows:

a. our policy was to favor an equation giving a satisfactory fit with the lowest number of parameters. In comparison with the four-parameter equations, the three-parameter Cox equation is less successful in describing the temperature dependence of $\Delta C'$ close to the triple point (see Fig. 1). The lower flexibility of the three-parameter equation seems, however, to be an advantage when fitting the higher members of the homologous series where the data are less numerous and of lower accuracy: four-parameter equations tend to become less reliable in the extrapolation of p_{sat}.

b. Our choice was influenced by the fact that the same procedure is being used for 1-alkanols where the four-parameter Cox equation is unquestionably superior to the Wagner equation and logically the description by the same type of relationship for both classes of compounds is preferable.

c. The Wagner equation requires knowledge of the critical parameters which can be only roughly estimated for the higher members of the homologous series due to thermal decomposition at lower temperatures.

d. In a wide temperature range reaching close to the triple point temperature the Wagner equation was less successful than the three-parameter Cox equation in describing the high quality vapor pressure data. This test was performed using results of Chirico and coworkers (89CHI/NGU) for decane which are probably the best data measured in the present class of compounds in the low and medium pressure range .

e. In an earlier study (79SCO/OSB) the Cox equation was found well suited for extrapolations of vapor pressures from the moderate pressure range down towards the triple point (without support of the thermal data). Our tests confirmed this finding and showed the three-parameter Cox equation was in this respect superior to the Wagner equation.

3. Methodology for the Simultaneous Correlation and for Establishing Recommended Values

3.1. Data Base

In order to avoid duplication of effort and to avoid conflicting recommendations, we have respected whenever

possible the IUPAC recommendations published recently for the individual properties (89AMB/WAL, 85MAJ/SVO, 91RUZ/ZAB). Our effort was concentrated on updating these recommendations when necessary and producing new evaluations at conditions where the previous recommendations were not quite satisfactory or were completely lacking.

Compiling and evaluating vapor pressures presented the most important part of effort in establishing the data base. Regarding the data in the medium pressure range (p_{sat} > 1 kPa), we have considered only those experimental sources which served for establishing the latest IUPAC recommendations (89AMB/WAL) complemented by more recent sources. On the other hand all available vapor pressures below 1 kPa were compiled.

Enthalpies of vaporization (direct calorimetric values) were taken from a data base of experimental values established during an IUPAC project; no significant new data have appeared in literature after publication of this compilation (85MAJ/SVO).

Unlike p_{sat} and ΔH_{vap}, the heat capacity difference ΔC°_{vap} cannot be considered as a direct experimental property: it was obtained from Eq. (2) where both heat capacity of ideal gas and that of the liquid were calculated from smoothing equations representing the recommended data. The ΔC°_{vap} values were calculated from a temperature close to the triple point up to the upper temperature limit of their inclusion in the simultaneous correlation.

All raw vapor pressure data were converted to the International Temperature Scale 1990 (ITS90), but no conversion was made for the thermal data as their likely errors always exceed the differences due to shifts between different temperature scales. More details on vapor pressures, thermal properties and auxiliary data used in the correlation are given in the Secs. 4 and 5.

3.2. Regression Method

The simultaneous correlation was performed by minimizing the objective function given in Eq. (15) by nonlinear least squares regression. The individual quantities with the superscript 'sm' were expressed from the following three equations. The logarithm of p_{sat} was obtained from Eq. (18) with $m = 2$

$$\ln\left(\frac{p_{sat}}{p_o}\right) = \left(1 - \frac{T_o}{T}\right)\exp\left(A_0 + A_1 T + A_2 T^2\right) \qquad (19)$$

using the normal boiling point as reference state (p_o = 101.325 kPa, $T_o = T_b$). Introducing this equation into the relationships (13) and (14) leads to

$$\Delta H' = R\exp\left(A_0 + A_1 + A_2 T^2\right)\left[T_o + T(T - T_o)(A_1 + 2A_2 T)\right] \qquad (20)$$

and

$$\Delta C' = RT\exp(A_0 + A_1 T + A_2 T^2)[2A_1 + 4A_2 T + (T - T_o)\cdot(2A_2 + A_1^2 + 4A_1 A_2 T + 4A_2^2 T^2)] \qquad (21)$$

To avoid distortions due to the uncertainty in the volumetric correction terms (see Eqs. 11 and 12), the thermal data were considered only at temperatures where the absolute values of differences $\Delta H' - \Delta H_{vap}$ and $\Delta C' - \Delta C^{\circ}_{vap}$ were smaller than, or comparable with, experimental errors in the enthalpy of vaporization and the heat capacity difference, respectively. In those cases where the thermal data reached into the region of medium vapor pressures, the upper temperature limits for their inclusion were typically 30 to 50 K below T_b for ΔH_{vap}, and 50 to 80 K for ΔC°_{vap}. For the lower members of the homologous series the thermal data were included up to the temperatures relatively close to T_b as the volumetric correction terms can be calculated with better accuracy (see Sec. 5.3). For *n*-alkanes C_{12} and higher, the thermal data were usually available only at conditions well below the normal boiling temperature where the effect of volumetric correction terms was negligible.

The regression was conducted in an iterative manner. In the first approximation, $\Delta H'$ and $\Delta C'$ were considered equal to ΔH_{vap} and ΔC°_{vap}, respectively, as at this stage no analytical expression for $p_{sat} = p_{sat}(T)$ was available yet and the volumetric correction terms in Eqs. (11) and (12) could not be properly calculated. In the next iterations the vapor pressures were described by the parameters obtained from the previous iteration. Usually five iterations were necessary to obtain the final fit.

3.3. Statistical Criteria

The individual data points were weighted using the expected uncertainties of the experimental data. The variances σ^2 of the individual data points were adjusted according to information in the original sources and taking into account consistency with the other data. The quantity $\sigma^2 \ln p_{sat}$ was obtained as a statistical estimate from the expected errors in temperature (σT) and pressure (σp)

$$\sigma^2 \ln p_{sat} = \left(\frac{\sigma p}{p}\right)^2 + \left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)^2_{sat}(\sigma T)^2 . \qquad (22)$$

Similarly $\sigma^2 \Delta C'$ was estimated from the expected errors in C_p° and C_p^{l} as

$$\sigma^2 \Delta C' = (\sigma C_p^{\circ})^2 + (\sigma C_p^{l})^2 . \qquad (23)$$

$\sigma^2 \Delta H'$ was obtained from the error in the enthalpy of vaporization as $\sigma^2 \Delta H' = (\sigma \Delta H_{vap})^2$. The effect of uncertainty in the volumetric correction terms (Eqs. 11 and 12) was neglected as their magnitude was in most cases smaller than the expected error in the thermal data.

The main criterion of the overall quality of correlation is the standard deviation of the fit

$$s_w = \left(\frac{S_{min}}{n-m}\right)^{1/2}, \quad (24)$$

where S_{min} denotes the value of the objective tion at its minimum, n denotes the overall number of data points (both for vapor pressure and the thermal data) and $m = 3$ is the number of adjustable parameters in the fitting equation. The main criterion for judging quality of the temperature fit for the individual properties ($X = p_{sat}$, ΔH_{vap} and ΔC°_{vap}) were their average weighted deviations d_w defined as

$$d_w = \left(\frac{\sum_{i=1}^{n_x}[(X^{exp} - X^{sm})/\sigma^2 X]_i^2}{n_x}\right)^{1/2}, \quad (25)$$

where n_x denotes the number of data points for a property. Additional statistical criteria used were: the average absolute deviation d, the average relative deviation d_r, the bias d_b and the difference between the number of data points with positive and negative deviation from the fit.

$$d = \left(\frac{\sum_{i=1}^{n_x}(X^{exp} - X^{sm})_i^2}{n_x}\right)^{1/2}, \quad (26)$$

$$d_r = \left(\frac{\sum_{i=1}^{n_x}[(X^{exp} - X^{sm})/X^{sm}]_i^2}{n_x}\right)^{1/2} 100, \quad (27)$$

$$d_b = \frac{\sum_{i=1}^{n_x}(X^{exp} - X^{sm})_i}{n_x}. \quad (28)$$

3.4. Correlation Procedure and Data Selection

Data fitting was realized in several steps.

1. Vapor pressures in the medium pressure range were fitted alone by Eq. (19) where p_o was put equal p_b = 101.325 kPa and A_0, A_1, A_2 and $T_o = T_b$ were adjustable parameters. In this way we obtained information about the scatter of medium vapor pressures and got the best possible fit in the range where p_{sat} measurements are the most reliable. The value of the normal boiling temperature obtained from this fit was considered as final and was not modified in the subsequent simultaneous correlation.

2. In the next step we correlated vapor pressures in the medium pressure range with the preselected thermal data (see Sec. 5.1 and 5.2) using p_0 and T_0 values determined in step 1. First the correlation weighting factors K_H and K_C were set at unity which gave the same weight to all data points regardless of which property they related to. These factors were changed when necessary to maintain a quality of p_{sat} fit in the medium pressure range comparable to that in step 1, while trying to keep the average weighted deviations d_w of the fit for ΔH_{vap} and ΔC°_{vap} near or below unity.

3. The low vapor pressures were compared on a deviation plot with the results of the fit under step 2. The individual p_{sat} sources were examined regarding their consistency with:

a. the low vapor pressure data from other sources
b. the thermal data
c. p_{sat} in the medium pressure range, provided the data overlapped or their limits were close to each other.

The low pressure p_{sat} to be included in the simultaneous correlation were selected and a new correlation was performed (see also Sec. 4.1.).

4. Consistency of the data in the homologous series was examined by producing several isobars between the triple and the normal boiling point describing the equilibrium temperature T_{eq} as a function of number of carbon atoms N. Smoothing of these data by a suitable equation allowed detection of possible systematic errors in the experimental data. Repeated simultaneous correlation with tentative omission of suspect data and subsequent isobaric plots helped to determine the source of error and which experimental information should be eliminated or which weights should be modified. At the same time this procedure served to generate the vapor pressure data by interpolation for those n-alkanes where no credible experimental information was available. Modifications in the data were made till the fits for all n-alkanes exhibited reasonable consistency over the whole homologous series.

5. The parameters from the final fit were used to generate the recommended values of vapor pressures and enthalpies of vaporization. The confidence intervals of the recommended p_{sat} and ΔH_{vap} values were estimated by a repeated correlation where the individual data sets were shifted by an increment corresponding to the expected errors of experimental data. The most unfavorable combination of these error effects was considered in the calculation of the total uncertainty of the recommended values (see detailed description in Sec. 6.3).

4. Vapor Pressures

4.1. Experimental Data

In compiling the vapor pressure data we have approached differently sources covering the medium pressure range only (p_{sat} > 1 kPa) from those containing all or part of their values in the low pressure range (p_{sat} < 1 kPa).

a. The data in the medium pressure range have been compiled and/or evaluated recently by several authors (84ESD1, 84ESD2, 85ESD, 86SAL/CAS, 89DAU/DAN, 89AMB/WAL); it did not seem, therefore, necessary to repeat the effort. We have taken over into our correlation the experimental data from the sources selected by Ambrose (92AMB) for producing the IUPAC recommendations (89AMB/WAL). It has to be mentioned that this data base differed to some extent from that used by Ambrose and Walton for the previous recommendations

in the ESDU Items (84ESD1, 84ESD2, 85ESD). In the case of C_6 to C_9 and C_{11} to C_{15} n-alkanes, the data obtained at the former National Bureau of Standards – NBS (today's National Institute of Standards and Technology – NIST) were considered, and in the case of pentane the later measurements by Osborne and Douslin (74OSB/DOU) were used. Two distinct data sets were presented in the NBS source for octane (45WIL/TAY), and we have included both of them. A different selection compared to Ambrose's choice of experimental data was made only in the case of decane where the NBS data (45WIL/TAY) were replaced with the recent ebulliometric measurements from the Bartlesville laboratory – NIPER (89CHI/NGU) as these data were considered superior. The ebulliometric data for eicosane from the same source were included (no experimental data in the medium pressure range were available for this compound at the time when Ambrose and Walton compiled the data). When establishing the IUPAC recommendations for C_{12} to C_{20} n-alkanes, Ambrose and Walton used in their correlation also some additional estimated data points. They were obtained by a procedure described by Ambrose and Sprake (70AMB/SPR) in which the equilibrium temperature was fitted in the homologous series as a function of carbon atom number at constant pressure. These estimated values were not included in our database. No experimental data source specifically covering the medium pressure range (p_{sat} > 1 kPa for all data points) was found in the literature for C_{17} to C_{19} n-alkanes.

b. The low vapor pressures of n-alkanes have not been evaluated in a systematic manner until now. We have compiled all available sources published after 1930 which reported data located fully or partly below the pressure limit of 1 kPa.

Table 2 reviews the data base of experimental vapor pressures. For each n-alkane the sources with data below 1 kPa are presented in chronological order, followed by the selected source of medium pressure data (all p_{sat} > 1 kPa) printed in italics as the last line in the section. When several distinct data sets were given for the same substance in one publication, there are several lines for one data source, each relating to one data set. The meaning of individual columns is as follows.

First column: name of substance

Second column: the abbreviated reference in the form YYAAA/BBBM, where YY are the last two digits of the year of publication, AAA and BBB are the first three letters of the last name of the first and second author (if present), respectively. M is a digit distinguishing papers with the same YYAAA/BBB code.

Third column: the total number of data points and the number of data points below 1 kPa are given left and right of the slash, respectively; symbol 'eqn' is used in those cases where only the parameters of a smoothing equation were presented in the original literature; symbol 's' denotes that the discrete values given in the original literature source were generated from a smoothing equation.

Fourth to seventh columns: lower and upper temperature limits of the data set in kelvin; lower and upper pressure limits (Pa).

Eighth and ninth columns: error in measurement of temperature and pressure as indicated in the original source; the uncertainty in temperature is given always in kelvin, pressure error is indicated either in pascals (Pa) or in percent (%); abbreviation 'nosp' is used when no specification is given in the original literature. Morgan (90MOR) gives for his data an analytical relationship for calculating the pressure error (see a note below Table 2). In several cases the overall error in vapor pressure is given in the literature; in this case the eighth column is empty and the pressure error in the ninth column includes also the propagated temperature error. In the case of two data sets reported in the paper by Chirico *et al.* (89CHI/NGU) the sign < was used to indicate that the overall error in vapor pressure was lower than the given maximum value relating to the upper temperature limit of experimental values.

Tenth column: purity of the substance in percent (given with the same number of significant digits as in the original source)

Eleventh and twelfth columns: type of the method used for determining the data and reference to the publication where the experimental setup is described. The coding used is as follows: 'sta' a static method, 'dyn' a dynamic (ebulliometric) method, 'sat' a gas-saturation (transpiration) method, 'ram' Ramsay-Young method, 'mas' measurement by mass spectroscopy, 'wef' a weighing effusion method, 'tef' a torsion effusion method. Description of techniques for measuring vapor pressure can be found in the review by Ambrose (75AMB).

4.2. Correlated Data

4.2.1. Medium Pressure Range

The data from the sources reporting p_{sat} in the medium pressure range were considered in correlation up to the normal boiling point or slightly above; the higher values of vapor pressures were omitted in order to get the best fit below T_b with the lowest number of parameters. This was the case for pentane (74OSB/DOU) and decane (89CHI/NGU), where 5 data points closest to the upper temperature limit of experiment were omitted. Similarly as in the original source the four highest data points (all at $T < T_b$) were omitted for eicosane in the ebulliometric data set from Bartlesville (89CHI/NGU); a considerably higher scatter of these values compared to that at lower temperatures indicated decomposition starting at temperature about 50 K below T_b. Several data points exhibiting larger than usual deviations from the smoothed values were eliminated in the NBS medium pressure data sets (temperatures in kelvin and pressures in kPa as given in the original data source are given in parenthesis): hexane (342.23,102.39), undecane (377.61,5.54; 437.19,43.03); dodecane (399.53,6.36; 404.26,7.66; 436.18, 23.44), tetradecane (428.01,5.53).

Morgan (90MOR) reported static measurements in a wide temperature range for the even-numbered C_{10} to C_{20} higher scatter of these values compared to that at lower temperatures indicated decomposition starting at temperature about 50 K below T_b. Several data points exhibiting larger than usual deviations from the smoothed values were eliminated in the NBS medium pressure data sets (temperatures in kelvin and pressures in kPa as given in the original data source are given in parenthesis): hexane (342.23,102.39), undecane (377.61,5.54; 437.19,43.03); dodecane (399.53,6.36; 404.26,7.66; 436.18, 23.44), tetradecane (428.01,5.53).

Morgan (90MOR) reported static measurements in a wide temperature range for the even-numbered C_{10} to C_{20} *n*-alkanes and nonadecane; his data covered mainly the medium pressure range and reached partly below 1 kPa. Consistency with the selected medium pressure sources was poor; differences for C_{14}, C_{16} and C_{20} *n*-alkanes often were more than 100 Pa at p_{sat} near and above 40 kPa. For that reason we decided to disregard completely this source despite the fact that the Morgan's measurements for octadecane and nonadecane were the only experimental data available above 5 kPa.

4.2.2. Low Pressure Range

In the low pressure region the scatter of data from different sources increases with decreasing vapor pressure, and differences between individual data sets were in some cases several tens of percent at pressures below 100 Pa. Presence of lower boiling impurities and/or insufficient degassing of samples can have a devastating effect on the results of measurements when approaching the triple point temperature. In many cases it is difficult to assess credibility of the data for making an appropriate choice; the selection was done following the procedure described in Sec. 3.4.

The best data available in the low pressure region are certainly those for decane and eicosane measured in the Bartlesville NIPER laboratory by the inclined piston method (89CHI/NGU). These data can be considered as reference data for higher *n*-alkanes.

Results for octadecane and eicosane measured by a gas-saturation method close to the triple point temperature have been reported by Macknick and Prausnitz (79MAC/PRA). The values for eicosane are reasonably consistent at their upper temperature limit with the data from the Bartlesville laboratory and were therefore also considered; on the other hand, the data for octadecane fit poorly in isobaric plots of $T_{eq} = T_{eq}(N_c)$. Vapor pressures for the latter substance below 1 kPa were reported by several authors and are relatively abundant, but are extremely scattered (see Fig. 17). For this reason no experimental p_{sat} data were considered for octadecane at all.

The Laboratory of Analytical Chemistry at the University Claude Bernard in Lyon (group of Professor Jose) reported in the recent years several data sets for C_{10} to C_{20} *n*-alkanes (86ALL/JOS1, 86ALL/JOS2, 92KAS, 93JOS), which more than doubled the number of data points available below 1 kPa. Above the pressure of 50 Pa the Lyon's datasets obtained for one compound with different samples and in some cases with different techniques (gas saturation versus static measurements) were self consistent within the claimed experimental errors, with the exception of octadecane. For decane and eicosane the Lyon data are consistent above 50 Pa to better than 5 percent with those from the Bartlesville laboratory. Most values reported at lower pressures seem to be, however, subject to significant uncertainties as differences between the individual Lyon data sets amounted often to more than 10 per cent. These findings led us to conclude that the Lyon datasets above 50 Pa can be candidates for inclusion for those compounds where Bartlesville data (obviously more reliable) were not available. After the simultaneous correlations of data for individual compounds were performed, the isobaric plots of $T_{eq} = T_{eq}(N_c)$ (see Eq. 34) showed good consistency in the case of C_{11} to C_{16} alkanes. Inconsistency was observed, however, for C_{17} to C_{19}. Therefore in the final correlation the Lyon data were included only for C_{11} to C_{16} *n*-alkanes between the temperature corresponding to the first p_{sat} data point above 50 Pa and the lower temperature limit of the selected medium pressure data. The statistical weight of the Lyon values, determined using information on accuracy from the authors (92JOS), was substantially lower compared to the selected medium pressure data and could not have any negative impact on the quality of the fit above the upper temperature limit of their inclusion.

No other datasets were included in the low pressure range as their credibility was not considered sufficient. The correlation for C_5 to C_9 *n*-alkanes was performed without any data points below 1 kPa; the values of Carruth and Kobayashi (73CAR/KOB) were obviously erroneous and data from other sources (see Table 2) were neither numerous nor trustworthy.

A large number of results grouped into the three separate data sets (according to the experimental technique used) were published recently for eicosane by Piacente and coworkers (91PIA/POM). The scatter of the data is, however, substantial and differences between the three sets and the Bartlesville data indicate a high probability of systematic errors (see Fig. 19b).

4.2.3. Final data selection

Considering the factors described above we preferred to ignore completely the experimental vapor pressures for C_{17} to C_{19} *n*-alkanes and all the p_{sat} data used in the correlation were obtained by an interpolation procedure using the isobaric $T_{eq} = T_{eq}(N_c)$ fits (see also Sec. 6.1.).

Tables 3 and 4 give quantitative information on how the individual data sets compare with the results of the simultaneous correlation. Deviation plots (Figs. 4 to 19) present a graphical comparison with the recommended data.

Vapor pressure data sets included in the simultaneous correlation are listed in Table 3 with the statistical

parameters indicating how the individual data sets compare with the final fit used for generating the recommended values. The following characteristics are presented:

First and second columns: the same meaning as in Table 2.

Third column: number of data points included in the correlation.

Fourth to seventh columns: temperature and pressure limits of the data included in the correlation.

Eighth and ninth columns: expected overall errors σp_{sat} in the vapor pressure at the lower and upper temperature limits of the included data; this value corresponds to the variance $\sigma^2 \ln p_{sat}$ used in the regression, see Eq. (15). The values are calculated using Eq. (22) from the errors in T and p reported in the data source (see Table 2, eighth and ninth columns) or were assigned by the evaluators in cases when this information was not available or the author's estimate did not seem to be realistic.

Tenth to fourteenth columns: average weighted deviation d_w, average deviation d, average percentage deviation d_r, bias of the data set d_b and the difference between the numbers of experimental points with positive and negative deviation. For definitions of these statistical characteristics see Sec. 3.3., Eqs. (25) to (28) with n_x equal to the number of the included experimental points in a given data series (column 3).

Table 4 listing statistical characteristics for the rejected data sets has a structure similar to the previous table (without columns four to nine). All listed statistical characteristics were determined using exclusively the vapor pressure values below 1 kPa.

5. Thermal and Other Data

5.1. Enthalpies of Vaporization

All experimental enthalpies of vaporization (calorimetric values) reported in literature before 1984 have been listed and assessed in a recent IUPAC publication (85MAJ/SVO). For inclusion into the simultaneous correlation we have made a selection of data sources which we considered reliable. Table 5 which reviews the included data sets has a structure similar to Table 3. The expected relative uncertainty σ_r of ΔH_{vap} in percent (column 8) was estimated by the compilers and served for calculating the variance $\sigma^2 \Delta H_{vap}$ used in Eq. (15). Note that the values in the third to the seventh columns indicate the ranges over which the data were included in the correlation. The upper limit of the entire range of experimental data for lower n-alkanes was in fact usually higher compared to that listed in Table 5; the data were, however, omitted at conditions where errors in the volumetric correction terms could distort the $\Delta H'$ values (see Eq. 11).

5.2. Heat Capacity Differences ΔC°_{vap}

Ideal gas heat capacities tabulated in the TRC tables (87TRC) served as a basis for the analytical description of the temperature dependence of C_p° using the relationship (81BUR/MAJ)

$$C_p^{\circ} = A + B_1 \frac{(C_1/T)^2 \exp(-C_1/T)}{(1-\exp(-C_1/T))^2} + B_2 \frac{(C_2/T)^2 \exp(-C_2/T)}{(1-\exp(-C_2/T))^2} . \quad (29)$$

The adjustable parameters A, B_1, B_2, C_1, C_2 valid at temperatures between 200 and 1000 K were established from 10 data points (all given the same statistical weight) by nonlinear least squares regression. The differences between the tabulated TRC values and those calculated from Eq. (29) were always below 0.1 percent, which is substantially less than the expected error of data (1 percent). For a listing of parameters A, B_1, B_2, C_1, C_2 see Table 6.

An evaluation of heat capacities for liquid n-alkanes C_1 to C_{18} was performed recently by Růžička *et al.* (91RUZ/ZAB). That publication lists all available data sources and the parameters of correlating cubic spline polynomials. The procedure used to establish the recommended values is in (91RUZ/ZAB) and will not be repeated here. The reliability of the C_p^l data in the region of the ΔC°_{vap} calculation was typically 0.5 percent or better with exception of C_{11}, C_{14} and C_{16} n-alkanes, where higher uncertainty was expected. In the case of C_{19} and C_{20} n-alkanes the calorimetric data were treated in an analogous way. For nonadecane experimental results were available between 305 and 453 K as a first degree polynomial in temperature with a stated accuracy of 1 percent (69ATK/LAR). Experimental data for eicosane (81HOE) were reported with very large error margin (5 percent); a plot of the calculated heat capacity differences confirmed that C_p^l values for eicosane must be in error.

The temperature dependence of ΔC°_{vap} for individual n-alkanes is illustrated in Fig. 2; dashed lines denote the parts of ΔC°_{vap} curves corresponding to temperature intervals where heat capacity values were eligible for inclusion (sufficiently low volumetric correction terms) but were not considered in the final correlation (see below). A review of the heat capacity differences ΔC°_{vap} included in the simultaneous correlation (n-alkanes C_5 to C_{16}) is presented in Table 7; for comparison all the characteristics are also given for ΔC°_{vap} of higher n-alkanes not considered in the final fit. Table 7 has an analogous structure to Tables 3 and 5. The values were generated in steps of 5 K. The lower temperature limit (column 3) is always close to the triple point and was limited only by the availability of experimental C_p^l data. For the upper temperature limit (column 4) of C_9 and C_{12} to C_{19} n-alkanes C_p^l data were available only at temperatures far below the normal boiling temperature. For the other n-alkanes liquid heat capacities were available up to temperatures where the volumetric correction terms in Eq. (12) become important; in this case the upper temperature limit for ΔC°_{vap} was set such that any danger of $\Delta C'$ distortion was quite small.

Exceptions to the policy regarding inclusion of ΔC°_{vap} values were made in the case of C_{14}, C_{16} and C_{20} n-alkanes. It is clear from Fig. 2 that the ΔC°_{vap} values generated

for eicosane are inconsistent with those for the lower members of the homologous series. As vapor pressure data of high quality were available for this compound close to the triple point it was possible to fit vapor pressures of eicosane alone without inclusion of any thermal data. An unrealistic temperature variation of ΔC°_{vap} is also apparent in the upper part of the temperature interval for hexadecane, probably due to errors in C_p^l, which are estimated to be 2 percent. Heat capacity differences were therefore included only up to 340 K compared to 413 K considered originally. In the case of tetradecane, omitting ΔC°_{vap} values at superambient temperatures where the uncertainty was large considerably improved the consistency over the homologous series (lower s_w of the $T_{eq} = T_{eq}(N_c)$ fit). The values were therefore considered only up to 298.5 K compared to 433.3 K used originally. Heat capacity differences were also not used for C_{17} to C_{18} *n*-alkanes, where the vapor pressure curves were obtained by interpolation.

The expected errors in ΔC°_{vap} at the lower and upper limit of the temperature range, in percent, are listed in columns 7 and 8 of Table 7. They were calculated from Eq. (23); in all cases the error limit for C_p° was set at 1 percent and that for C_p^l was adjusted according to indications given in (91RUZ/ZAB).

5.3. Auxiliary Data

5.3.1. Second Virial Coefficients

The second virial coefficient B and its first and second temperature derivatives were required for expressing the volumetric correction terms in Eqs. (11) and (12). They played a role in the correlations for *n*-alkanes up to C_{11}; for the higher members of the homologous series vapor pressures corresponding to the available temperature range for ΔH_{vap} and ΔC°_{vap} were sufficiently low to make the volumetric correction terms insignificant. An analytical description of B versus T was needed at conditions below the normal boiling temperature where experimental data on second virial conditions were limited. Dymond (86DYM) and Tsonopoulos *et al.* (89TSO/DYM) have evaluated literature data on B values for *n*-alkanes. They supplied recommendations based on experimental data up to C_8 and examined different methods for predicting B for the higher members of the homologous series where no experimental data have been reported. For our particular case use of the generalized Tsonopoulos prediction method seemed to be the best option (74TSO). This technique is considered as one of the most successful and reproduces the second virial coefficients of *n*-alkanes within their experimental errors (89TSO/DYM). The second virial coefficient of hydrocarbons was therefore calculated from the following equations

$$B = \frac{RT_c}{p_c}\left[f_0(T_r) + \omega f_1(T_r)\right], \tag{30}$$

$$f_0(T_r) = 0.14445 - \frac{0.33}{T_r} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} - \frac{0.000607}{T_r^8}, \tag{31}$$

$$f_1(T_r) = 0.0637 + \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8}. \tag{32}$$

Values of the critical parameters T_c and p_c and acentric factors ω were taken from the recent DIPPR tables (92DIP) and are listed in Table 8.

The advantage of the Tsonopoulos technique is particularly its ability to extrapolate reasonably well below the normal boiling temperature. The Tsonopoulos method is an extension of the technique by Pitzer and Curl (57PIT/CUR) which was developed by considering as experimental input also the difference between the heat capacity of vapor and that of ideal gas. This quantity was determined for several lower *n*-alkanes by flow calorimetry and is directly related by Eqs. (8) and (9) to the second temperature derivative of B. It can therefore be expected that the predictions of the temperature derivatives of the second virial coefficient will be reasonable.

5.3.2. Molar Volumes of Liquid

Molar volumes of the liquid phase V^l along the saturation line and its first and second temperature derivatives play a very minor role in Eqs. (11) and (12). Thus the means by which they are calculated is not important and will not be discussed in detail here. Martin's equation describing the saturated molar volume of liquid up to the critical point was used

$$V^l = \frac{V_c}{\sum_{i=0}^{5} A_i\left(1 - \frac{T}{T_c}\right)^{i/3}} \tag{33}$$

with parameters reported by Cibulka (93CIB).

5.3.3. Triple Point Temperatures

Slightly differing triple point temperatures have been reported in the literature. In some cases it is not clear whether the triple point temperature T_t or rather the melting point temperature T_m (relating to the atmospheric pressure and presumably an air saturated sample) are listed. The difference between the two temperatures is due to the effect of pressure and the dissolved air; generally T_m is a few hundredths of a kelvin below T_t. For *n*-alkanes the differences between T_m and T_t are less than 0.02 K, which is comparable with the uncertainty of various data sources reporting experimental values. The accurate determination of this difference would require very careful measurements on samples of high purity; as such high quality measurements are not available it is preferable to set $T_m = T_t$

We have decided to use the temperatures reported from the predecessor of the NIPER laboratory in Bartlesville (67MES/GUT) as these values are better

Bartlesville (67MES/GUT) as these values are better defined compared to those from other secondary sources; all values were converted from the IPTS-48 to the ITS-90 scale.

6. Recommended Values

6.1. Consistency of the Data over the Homologous Series

The simultaneous correlation was first performed for each substance separately except for C_{17} to C_{19} *n*-alkanes where all vapor pressures were discarded (see Sec. 4.2.). Subsequently the isobaric fits of temperature versus the number of carbon atoms were made for all *n*-alkanes at 21 pressures: 0.1, 0.5, 1, 5, 10, 50, 100, 250, 500, 1000, 2500, 5000, 7000, 10000, 20000, 30000, 40000, 50000, 65000, 80000, 101325 Pa. A relationship

$$T_b = \frac{\sum_{i=0}^{n} a_i N_c^i}{1 + \sum_{j=1}^{m} b_j N_c^j} \qquad (34)$$

with four adjustable parameters was found to be the best suited for this type of dependence and clearly superior to a third degree polynomial. A satisfactory fit was obtained with four parameters ($n=1$, $m=2$). The parameters were obtained by nonlinear least squares regression using the weighting factors based on the expected uncertainty in the recommended vapor pressures (see below) converted to errors in temperature. This type of fitting across the homologous series enabled the discovery of an inconsistency for tetradecane which was corrected by omitting the lowest values of p_{sat} in the medium pressure range and a part of the ΔC_{vap}° values. It also showed that available vapor pressures for C_{17} to C_{19} were probably subject to serious errors and had to be eliminated. After performing a new simultaneous correlation for tetradecane with the modified input data, the vapor pressures for the above three compounds were calculated from the isobaric fits based on the final values for C_5 to C_{16} and C_{20} *n*-alkanes. The interpolated p_{sat} values were finally fitted for each substance separately by the Cox equation. Thermal data for C_{17} to C_{19} were not included in the final fits as they were of low quality and in the case of the simultaneous treatment the results were not quite consistent with the isobaric fits in the lower part of the vapor pressure curve. Provided the proper weights reflecting the expected errors in the interpolated vapor pressures and thermal data were used, the inclusion of ΔC_{vap}° into the correlation would have shifted the vapor pressures near the triple point temperature by 4, 5 and 10 per cent for C_{17}, C_{18} and C_{19} *n*-alkanes, respectively, compared to the simple fit of interpolated vapor pressures. Our preference was to maintain good consistency over the whole homologous series.

The good quality of the isobaric fits is documented in Table 9. The table lists for several pressures the differences between the temperatures obtained from isobaric plots (Eq. 34) and those calculated from the Cox equation (Table 12); the corresponding pressure difference (the listed pressure minus the pressure obtained from the Cox equation using the temperature generated by Eq. 34) is given in parentheses. Comparison of these pressure differences with expected uncertainty of the selected experimental vapor pressures above 1 kPa (see values of σ_{min}, σ_{max} in Table 3) and with the estimated error limits of extrapolated values below 1 kPa (Figs. 4 to 19) indicates that the isobaric fits are able to reproduce p_{sat} data within the accuracy of the recommended values. This suggests good consistency of data over the whole homologous series.

Vapor pressures for eicosane were not included into the isobaric fits above 50 kPa where no experimental data were included in the correlation with the Cox equation (decomposition at higher temperatures). This means that data for the C_{17} to C_{19} *n*-alkanes were obtained above this pressure by extrapolation; we do not think, however, that any important distortion is likely to occur. Our belief is supported by the two following findings:

1. The normal boiling temperature for eicosane extrapolated from the Cox equation differs from that obtained using the isobaric extrapolation by 0.08 K; this is reasonable agreement, suggesting consistency of both extrapolation procedures. If the isobaric plots had been constructed using only the data for C_{10} and higher *n*-alkanes, the difference in T_b would have been only 0.003 K.
2. Extrapolations of p_{sat} to octacosane using isobaric fits gave satisfactory agreement with the results reported recently by Chirico *et al.* (89CHI/NGU) over the whole experimental interval. Differences were −14 and 4 per cent in pressure at the lower and upper limit of the data; 453 to 575 K (corresponding to p_{sat} of octacosane ranging from 13.1 to 3885 Pa).

6.2. Results of the Simultaneous Correlation

The parameters of the Cox equation (Eq.19) for the final fit of all C_5 to C_{20} *n*-alkanes are listed in Table 10. Beside the three adjustable parameters, the reference pressure p_o and the reference temperature T_o are given at the normal boiling conditions (the way of determining T_o and p_o is described in Sec. 3.4.). The three decimal digits for T_b are required because of numerical considerations and do not express the real accuracy. It should be noted that the parameters are valid for the temperature range delimited by the triple and normal boiling temperature. The equations allow a short extrapolation above T_b but should not be used for extrapolating towards the critical point.

Statistical characteristics of the final fit are given in Table 11. The following quantities are listed: the overall standard weighted deviation of the fit (Eq. 24), the average weighted deviations (Eq. 25) for the three correlated properties and the correlation factors K_H and K_C (see Eq. 15). It is apparent that all three properties were fitted in most cases within the expected error limits. As

expected, the average weighted deviations of p_{sat} were exceptionally low for C_{17} to C_{19} hydrocarbons where the interpolated data rather then raw experimental values were used as input. Some inconsistency of p_{sat} and ΔC°_{vap} data was observed for heptane, nonane and decane; fornonane both K_H and K_C correlation factors had to be changed from unity in order to improve the fit of the thermal data.

The last two columns in Table 11 were included to show quantitatively how the simultaneous correlation affects the fit of the highly accurate medium vapor pressure data. For each *n*-alkane both columns list the average absolute deviations *d* for the set of the selected medium vapor pressures (NBS or Bartlesville data). The penultimate column relates to the simultaneous fit of this set with all the other data included in the correlation (values are identical with those in the eleventh column of Table 3); the last column lists *d* for a separate correlation of the selected medium vapor pressures only, without considering any additional data. Comparison of these two columns indicates that the simultaneous treatment of several types of data did not significantly lower the quality of the fit for the medium vapor pressures. Substantial differences were observed only for *d*'s of eicosane indicating some inconsistency between the medium and low vapor pressures (no thermal data were considered in the final fit for this compound). Large standard deviations s_w and d_w were also observed for this compound indicating that differences between experimental and smoothed values were substantially higher than expected errors which served for calculating $\sigma^2 \ln p_{sat}$ used in Eq. 15. Chirico *et al.* reported in their paper (89CHI/NGU) extremely low values of σp_{sat}, which we also used in our fitting (see Table 3). Correlation in this publication is, however, practically identical with Chirico *et al.* who also used the Cox equation (both representations are identical to 1 and 0.1 Pa for the ebulliometric and static data sets, respectively). The inclusion of the data by Macknick and Prausnitz near the triple point did not alter the fit at higher pressures.

The enthalpy of vaporization can be obtained at any temperature between T_t and T_b by combining Eqs. (11) and (20) using the parameters in Table 10 with volumetric terms calculated from Eqs. (30) to (33). Tables 12 and 13 list for several isobars the equilibrium temperatures and corresponding enthalpies of vaporization, respectively. The recommended values of ΔH_{vap} at T_b from the IUPAC evaluation (85MAJ/SVO) of calorimetric enthalpies of vaporization are given in parentheses in the last column of Table 13 for C_5 to C_8 and C_{10} *n*-alkanes. The difference of over 2 per cent for decane indicates a probable systematic error in the calorimetric measurement which was originally evaluated by Majer and Svoboda as accurate to 1 per cent. Recommended values of p_{sat}, ΔH_{vap} and ΔC°_{vap} at the triple point temperature and 298.15 K are listed in Tables 14 and 15, respectively. The values of $\Delta H'$ and $\Delta C'$ calculated from Eqs. (20) and (21) are also listed at 298.15 K; their difference from ΔH_{vap} and ΔC°_{vap} illustrates how the size of volumetric correction terms (Eqs. 11 and 12) decreases with increasing length of the carbon chain for the given temperature.

6.3. Analysis of Possible Errors and Reliability of Recommended Values

6.3.1. Vapor pressures

Evaluating the accuracy of the recommended vapor pressures is relatively easy in the medium pressure range where reliable data are available and the influence of the thermal data is limited. The uncertainty of p_{sat} generated from the Cox equation is comparable with the expected error of the experimental data from the selected medium pressure sources. Concrete values are given for the lower and upper temperature limits of data in Table 3 (σ_{min}, σ_{max}): in the case of eicosane the uncertainty is about twice as high (1 and 5 Pa at the temperature limits). The normal boiling temperatures are expected to be reliable to ± 0.01 K for C_5 to C_{12} *n*-alkanes and to ± 0.02 K for C_{13} to C_{16} *n*-alkanes. For higher *n*-alkanes the accuracy of T_b is believed to be ± 0.05 K for heptadecane and decreases with the increasing number of carbon atoms due to increasing probability of the compound decomposition at high temperature.

The estimation of accuracy is more complex in the low pressure range. The experimental p_{sat} data when included (all data were omitted for C_5 to C_9 *n*-alkanes) were fitted with a much lower statistical weight compared to those in the medium pressure range. Thermal data had therefore a substantial effect on the results of the correlation with the exception of C_{10} and C_{20} *n*-alkanes for which also the p_{sat} data below 1 kPa were included with a high statistical weight (no thermal data were considered for eicosane at all). In most cases the recommended values in the low pressure range depend on vapor pressures, thermal data, their weighting during correlation and their respective location over the temperature range of correlation. In the regions where p_{sat} data are missing or have low statistical weight, the results are to some extent also affected by the form of the vapor pressure equation used. A more general analysis of all the factors playing a role in the simultaneous correlation is given elsewhere (94RUZ/MAJ); results of several tests performed for C_5 to C_{16} *n*-alkanes are given below. When not otherwise indicated, all of the following quantitative information relates to the triple point, where the impact of the above factors is most pronounced.

a. Using identical input data, the simultaneous correlation was repeated with two four-parameter vapor pressure equations used previously in literature for the extrapolation controlled by thermal data (Eq. 16 with *k* changing from 0 to 2, and the Wagner Eq. 17). Compared to the three-parameter Cox equation, these two equations gave in average the vapor pressures by 4.4 and 2.0 percent higher (with the exception of decane where p_{sat} was 2.4 and 1.6 per cent lower), respectively. This comparison illustrates by how much the behavior of the correlation equations might change depending on whether

accurate vapor pressures near the triple point temperature are available.

b. For each n-alkane the effect of uncertainty in the vapor pressures and thermal data was examined by shifting the selected values of p_{sat}, ΔH_{vap} and ΔC°_{vap} by their respective error limits and repeating the simultaneous correlation. Such a simulation permitted estimation of the effect of errors in the individual input properties on the vapor pressure curve below 1 kPa. The shift in p_{sat} changed the vapor pressure at T_t by on average 0.5 and 3.9 per cent for C_5 to C_{10} and C_{11} to C_{16} n-alkanes, respectively; the maximum change was observed for tetradecane (6.1 percent). Similarly for all C_5 to C_{16} n-alkanes the shifts in ΔH_{vap} and ΔC°_{vap} caused average changes in p_{sat} at T_t of 0.6 and 4.0 per cent, respectively; the maximum change was observed in the case of ΔH_{vap} shift for tetradecane (1.9 percent) and in the case of ΔC°_{vap} shift for undecane (6 percent).

c. The test described under b. was repeated with the two equations used in the test a. to see if there were any differences in sensitivity of the various correlation equations to errors in the input data. The changes corresponding to shifts in p_{sat}, ΔH_{vap} and ΔC°_{vap} were, usually, within 2 percent, identical with those determined with the three-parameter Cox equation, thus indicating a similar sensitivity for the three equations.

Figures 4 to 19 present the deviations of the experimental data below 1 kPa from the recommended values; the triple point temperature is marked on the temperature axis by a triangle. Two plots are given for eicosane where a large number of data were reported in literature differing substantially from each other. The full lines below and above the zero deviation axis delimit the maximum uncertainty 'tunnel' of the recommended data. Estimation was based on the procedure described under b. Fitting was performed repeatedly with the p_{sat}, ΔH_{vap} and ΔC°_{vap} data simultaneously increased and/or decreased by their respective error limits. All eight possible combinations of plus and minus shifts were examined in order to determine the maximum change in vapor pressure $(\delta p_{sat})_{max}$. The uncertainty limits in percent $(\Delta p_{sat})_r$ were calculated from the formula

$$\left(\Delta p_{sat}\right)_r = \left(\frac{1.5(\delta p_{sat})_{max}}{p_{sat}}\right)100 \qquad (35)$$

the factor of 1.5 being used as an allowance for unaccounted sources of uncertainty (effect of the equation type to the results of extrapolation etc.). In the case of C_{17} to C_{19} n-alkanes the uncertainty 'tunnel' was calculated from the error margins of the interpolated data points which were estimated by considering the accuracy of the recommended p_{sat} data for the nearest neighbors (C_{15},C_{16},C_{20} n-alkanes).

6.3.2. Enthalpy of vaporization

Calorimetric enthalpies of vaporization were included, in the correlation for n-alkanes up to C_{16} at one temperature or over a limited temperature range (several tens of degrees) starting from 298.15 K where measurements were most frequent (see Table 5). In the interval where calorimetric results were considered, the uncertainty of the recommended ΔH_{vap} is comparable to and in some cases better than that of the included calorimetric values (see Table 5). Inconsistency was observed only for nonane at 298.15 K; the calculated ΔH_{vap} for decane were certainly superior to the calorimetric values (63COU/KOZ).

In the region where calorimetric ΔH_{vap} were not included, the recommended data above 1 kPa depend mainly on the quality of the selected experimental vapor pressures. Close to the normal boiling temperature the reliability is also affected by the accuracy of the volumetric correction term (Eq. 11). The Tsonopoulos method is, however, very reliable for n-alkanes at least up to decane; therefore, the recommended enthalpies of vaporization near T_b are not impaired significantly by the uncertainty in the second virial coefficient. It can be expected that between 1 kPa and 100 kPa the error in ΔH_{vap} is below 0.5 and 1 percent for C_5 to C_{10} and C_{11} to C_{16} n-alkanes, respectively; for the C_{17} to C_{19} n-alkanes the probable error is below 2 percent. In the case of eicosane the recommended enthalpies of vaporization are accurate to 0.5 percent in the range from 500 to 600 K where the calculation is based on ebulliometric vapor pressures of high quality; uncertainty is higher above this temperature because of probable substance decomposition.

In the region below 1 kPa, estimating the reliability of recommended values is somewhat complex, especially when few or no experimental ΔH_{vap} values were considered. An analysis similar to that described in the previous paragraph was used to evaluate how the recommended values can be affected by the quality of input data and their distribution over the vapor-liquid saturation line. The calculated enthalpies of vaporization are less sensitive to the shifts in input quantities compared to vapor pressures; the results are affected primarily by ΔC°_{vap} with the effect increasing with the increasing extrapolation length. At the triple point temperature the expected error is 0.5 and 1 percent higher compared to that in the region above 1 kPa for C_5 to C_9 and C_{11} to C_{18} n-alkanes, respectively. For decane and eicosane the error is likely to be below 0.5 percent due to the availability of exceptionally good vapor pressure measurements below 1 kPa.

6.4. Comparison with Previous Evaluations

Tables 16 and 17 show how the p_{sat} data from the five major previous evaluations compare with the vapor pressures recommended in this publication (all data were converted to ITS90). The tabulated differences (in percent or Pa) are the vapor pressures calculated at the temperatures given in Table 12 (using the equation in the listed source) minus the pressure in the header. In the medium pressure range the p_{sat} values reported in the five listed evaluations are always closely related to the NBS measurements made for the API Research Project 44.

This means that our selected experimental data for the medium pressure range are practically identical with those derived in the previous evaluations for C_6 to C_9 and for C_{11} to C_{16} *n*-alkanes. The individual evaluations differ mainly in the way the data were correlated and how the recommended values in the low pressure range were obtained. King *et al.* (74KIN/ALN, 86KIN/MAH) and Ambrose and Davies (80AMB/DAV) used the simultaneous correlation of p_{sat} with the thermal data to obtain recommended values down to the triple point temperature. The procedure for obtaining the data in the low pressure range was not specified for the other secondary sources (87TRC, 89DAU/DAN and 92DIP data).

Unlike in our approach, King and coworkers did not adjust all parameters simultaneously but proceeded stepwise integrating twice the first degree polynomial $\Delta C' = RA_{1n} + 2RA_2T$ to get Eq. (16) in its four-parameter form ($k = 0, 1, 2$). The first two parameters were determined exclusively from the ΔC°_{vap} data, A_0 was obtained from the calorimetric ΔH_{vap} at 298.15 K and A_1 from the vapor pressures close to T_b. The database used differed to some extent from ours, especially regarding ΔC°_{vap} values, API44 p_{sat} values were used as input in the medium pressure range.

Ambrose and Walton (89AMB/WAL) used the Wagner equation to correlate simultaneously vapor pressures from several sources in order to get a description of p_{sat} with a single set of parameters between the triple and critical points. Vapor pressures below 10 kPa obtained by King and Al-Najjar (74KIN/ALN) for C_6 to C_{10}, C_{12}, C_{14} and C_{16} *n*-alkanes were also included in the fits; for that reason both sources exhibit similar deviations from our recommendations at low pressures. Isobaric interpolation by a polynomial was used to obtain the low pressure data for other members of the homologous series.

Data presented in the TRC tables (87TRC), based mainly on the API Research Project 44, are listed as parameters of the Antoine equation valid over a limited temperature range. Two distinct sets of parameters were used to calculate the temperatures at five pressures up to 1 kPa, and at two higher pressures. While agreement with our values is reasonable in the medium pressure range, the TRC recommendations are obviously erroneous for most *n*-alkanes in the low pressure range.

Vapor pressure recommendations published by Daubert and Danner (89DAU/DAN) are identical with the data of the Design Institute for Physical Property Data – DIPPR 801 Tables from 1988. They are based on a combination of the API44 values with additional data from both primary and secondary sources. The recommended data are presented as parameters of a five-parameter relationship based on Eq. (16) with k changing from 0 to 2 with one additional adjustable parameter in the exponent. Agreement with our recommendations is surprisingly poor both at low and medium pressures indicating serious problems of this evaluation.

During the revision of this article after the review we have received new improved DIPPR 801 data (92DIP), where the agreement with our recommendations was generally better with exception of C_6, C_{15} and C_{18} *n*-alkanes where substantial differences persist both at low and medium pressures. As our recommended values are reasonably consistent over the homologous series, the last DIPPR data for these three *n*-alkanes should be reexamined. At the normal boiling point the differences for C_8 to C_{19} *n*-alkanes between the DIPPR values and our recommendations (which are in good agreement with Ambrose and Walton) are larger than one would expect. The probable reason is that the equation used by DIPPR for describing the whole vapor-liquid saturation line is not flexible enough for fitting satisfactorily the accurate measurements near 100 kPa.

Our recommendations for C_5 to C_{16} *n*-alkanes are closest to those of Ambrose and Walton which seem to be superior to the other sources for these compounds. Particularly, in the medium pressure range the differences are close to the error margins of the experimental data with the exception of tetradecane. In the low pressure range our recommendations represent a refinement especially for C_{11} to C_{16} *n*-alkanes.

It is apparent from Tables 16 and 17 that the differences between the recommended values from this publication and those from the evaluations published before 1990 are especially important for C_{17} to C_{20} *n*-alkanes. Our recommendations are much better founded as they benefited from the accurate new data for eicosane (89CHI/NGU), which improved significantly the reliability of the recommendations for C_{17} to C_{19} *n*-alkanes where all the data were obtained by interpolation.

TABLE 1. Effect of the volumetric correction terms on calculating $\Delta H'$ and $\Delta C'$ from thermal data (*n*-heptane)

T	p	ΔH_{vap}	$\Delta H'$	Dif.	ΔC°_{vap}	$\Delta C'$	Dif.
K	Pa	kJ·mol^{-1}		%	J·mol^{-1}·K^{-1}		%
233.15	7.63E+1	40.87	40.88	0.0	−68.91	−68.26	−0.9
253.15	3.93E+2	39.50	39.55	0.1	−66.37	−64.77	−2.4
273.15	1.52E+3	38.18	38.29	0.3	−63.84	−60.51	−5.2
293.15	4.73E+3	36.89	37.13	0.7	−61.49	−55.55	−9.7
313.15	1.23E+4	35.61	36.08	1.3	−59.36	−49.92	−15.9
333.15	2.81E+4	34.34	35.14	2.3	−57.33	−43.63	−23.9
353.15	5.71E+4	33.06	34.34	3.9	−55.22	−36.69	−33.6
373.15	1.06E+5	31.77	33.68	6.0	−52.95	−29.08	−45.1

TABLE 2. Review of experimental vapor pressure data

All sources reporting vapour pressures below 1 kPa are listed, the selected medium pressure source (all p_{sat} > 1 kPa) is listed in italics

Alkane	Reference	No. pts.	T_{min} K	T_{max}	p_{min} Pa	p_{max}	Error in T/K	Error in p	Purity %	Method	Reference
pentane	40MES/KEN	13/1	208.0	298.0	4.1E+2	6.8E+4	nosp	nosp	99.961	nosp	
	51TIC/LOS	13/12s	147.5	223.4	1.3E-1	1.3E+3	0.3	nosp	99.85	mas	51TIC/LOS
	73CAR/KOB	10/8	143.6	242.3	8.1E-2	3.4E+3		3 %	99.90	sat	73CAR/KOB
	75HOR/HOP	49/2	216.0	296.6	8.0E+2	6.4E+4	nosp	nosp	99.98	sta	75HOP/PAR
	74OSB/DOU	*15/0*	*268.8*	*341.4*	*2.0E+4*	*2.7E+5*	*0.001*	*nosp*	*99.98*	*dyn*	*66OSB/DOU*
hexane	64WOL/HOP	4/1	233.2	293.1	4.9E+2	1.6E+4	nosp	nosp	nosp	sta	62WOL/HOP
	65WOL/HOP	9/3	218.2	293.1	1.3E+2	1.6E+4	nosp	nosp	nosp	sta	62WOL/HOP
	66WOL/HOP	5/2	223.2	293.1	2.9E+2	1.6E+4	0.02	1 Pa	99.96	sta	62WOL/HOP
	68WOL/WUR	5/2	223.2	293.1	2.4E+2	1.6E+4	nosp	nosp	99.96	sta	62WOL/HOP
	73CAR/KOB	12/9	177.7	264.9	1.4E+0	3.1E+3		3 %	99.95	sat	73CAR/KOB
	45WIL/TAY	*16/0*	*286.2*	*342.7*	*1.2E+4*	*1.0E+5*	*0.002*	*5 Pa*	*99.9991*	*dyn*	*45WIL/TAY*
heptane	73CAR/KOB	10/7	185.3	295.6	2.9E-1	5.1E+3		3 %	99.92	sat	73CAR/KOB
	49FOR/NOR	*20/0*	*299.2*	*372.4*	*6.4E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.94*	*dyn*	*45WIL/TAY*
octane	31LIN	3/3	263.9	276.8	2.0E+2	4.9E+2	nosp	nosp	nosp	ram	31LIN
	58COO	3/1	273.1	308.1	3.6E+2	3.2E+3	nosp	nosp	nosp	sta	58COO
	73CAR/KOB	10/8	216.6	297.1	2.4E+0	1.6E+3		3 %	99.85	sat	73CAR/KOB
	45WIL/TAY	*29/0*	*326.0*	*399.7*	*7.7E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.9996*	*dyn*	*45WIL/TAY*
nonane	64WOL/HOP	3/3	253.2	293.1	2.7E+1	4.5E+2	nosp	nosp	nosp	sta	62WOL/HOP
	73CAR/KOB	10/10	219.7	307.7	7.6E-1	7.2E+2		3 %	99.68	sat	73CAR/KOB
	79SCH/RAL	2/1	302.2	324.5	8.0E+2	2.9E+3	nosp	nosp	nosp	dyn	58SCH/RAL
	49FOR/NOR	*20/0*	*343.5*	*424.9*	*6.4E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.94*	*dyn*	*45WIL/TAY*
decane	31LIN	4/4	269.4	281.6	2.2E+1	6.3E+1	nosp	nosp	nosp	ram	31LIN
	73CAR/KOB	8/8	243.5	310.6	1.7E+0	2.1E+2		3 %	99.85	sat	73CAR/KOB
	86ALL/JOS1	11/6	298.1	347.9	1.8E+2	3.2E+3	0.02	1 %	nosp	sat	86ALL/JOS1
	89CHI/NGU	12/9	268.1	348.1	1.7E+1	3.2E+3		<1 Pa	99.998	sta	65DOU/OSB
	90MOR	16/1	323.1	588.1	8.7E+2	1.4E+6	0.03	note	99.85	sta	90MOR
	93JOS	39/14	244.0	467.4	1.5E+0	1.6E+5	0.02	2 %	98+	sta	88SAS/JOS
	89CHI/NGU	*21/0*	*373.2*	*490.3*	*9.6E+3*	*2.7E+5*	*0.001*	*<10 Pa*	*99.998*	*dyn*	*65DOU/OSB*
undecane	92KAS	20/9	253.5	453.3	8.3E-1	3.9E+4	0.02	2 %	98+	sta	88SAS/JOS
	93JOS	46/11	254.3	468.9	1.1E+0	1.0E+5	0.02	2 %	98+	sta	88SAS/JOS
	55CAM/ROS	*20/0*	*377.6*	*470.4*	*5.5E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.97*	*dyn*	*45WIL/TAY*
dodecane	51TIL/PES	1/1	355.1		7.2E+2		nosp	nosp	nosp	nosp	
	86ALL/JOS1	19/17	298.1	389.6	1.7E+1	4.3E+3	0.001	1Pa	99.5	sta	86ALL/JOS1
	86ALL/JOS2	5/5s	302.1	352.0	2.4E+1	6.9E+2	0.001	1Pa	99.5	sta	84MIC/JOS
	88SAS/JOS	37/33	263.9	371.2	5.9E-1	1.8E+3	0.02	2 %	98+	sta	88SAS/JOS
	90MOR	13/1	353.1	588.1	7.3E+2	6.7E+5	0.03	note	99.94	sta	90MOR
	92KAS	17/9	273.5	453.3	1.9E+0	3.9E+4	0.02	2 %	98+	sta	88SAS/JOS
	93JOS	36/11	263.7	467.5	6.4E-1	5.8E+4	0.02	2 %	98+	sta	88SAS/JOS
	45WIL/TAY	*20/0*	*399.5*	*490.5*	*6.4E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.9994*	*dyn*	*45WIL/TAY*
tridecane	51TIL/PES	1/1	356.2		4.0E+2		nosp	nosp	nosp	nosp	
	93JOS	33/12	273.6	467.4	4.8E-1	3.5E+4	0.02	2 %	98+	sta	88SAS/JOS
	55CAM/ROS	*14/0*	*412.5*	*509.2*	*5.5E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.92*	*dyn*	*45WIL/TAY*
tetradecane	31LIN	1/1	292.1	292.1	0.9E-2	0.9E-2	nosp	nosp	nosp	ram	31LIN
	51TIL/PES	1/1	379.9		6.7E+2		nosp	nosp	nosp	nosp	
	86ALL/JOS1	6/5	343.1	394.7	7.2E+1	1.3E+3	0.02	1 %	nosp	sat	86ALL/JOS1
	90MOR	16/1	373.1	588.1	4.4E+2	3.4E+5	0.03	note	99.95	sta	90MOR
	93JOS	34/12	284.0	467.1	4.1E-1	2.1E+4	0.02	2 %	98+	sta	88SAS/JOS
	55CAM/ROS	*11/0*	*428.0*	*527.3*	*5.5E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.93*	*dyn*	*45WIL/TAY*
pentadecane	86ALL/JOS1	6/5	333.1	409.1	1.6E+1	1.3E+3	0.02	1 %	nosp	sat	86ALL/JOS1
	93JOS	21/12	293.8	467.4	3.6E-1	1.3E+4	0.02	2 %	98+	sta	88SAS/JOS
	55CAM/ROS	*10/0*	*442.8*	*543.6*	*5.5E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.93*	*dyn*	*45WIL/TAY*

TABLE 2. Review of experimental vapor pressure data – Continued

All sources reporting vapour pressures below 1 kPa are listed, the selected medium pressure source (all p_{sat} > 1 kPa) is listed in italics

Alkane	Reference	No. pts.	T_{min} K	T_{max} K	p_{min} Pa	p_{max} Pa	Error in T/K	Error in p	Purity %	Method	Reference
hexadecane	49BRA/SHE	eqn.	293.1	308.1	1.2E-1	6.2E-1	nosp	nosp	nosp	wef	46BRA/EVA
	49PAR/MOO	6/6	299.1	323.1	2.2E-1	2.3E+0	nosp	5 %	nosp	wef	49PAR/MOO
	51TIL/PES	1/1	400.5		4.0E+2		nosp	nosp	nosp	nosp	
	55MYE/FEN	26/8s	354.1	559.1	2.7E+1	1.0E+5	0.2	nosp	nosp	dyn	55MEY/FEN
	69EGG/SEI	10/10	299.0	413.1	2.1E-1	8.2E+2	nosp	nosp	nosp	sat	68EGG/JOK
	81GRE/POT	4/3	357.8	417.7	3.6E+1	1.2E+3	0.1	nosp	nosp	sat	77GRE/BON
	87MIL/FEN	11/2	388.9	560.2	2.5E+2	1.0E+5	nosp	nosp	nosp	dyn	87MIL/FEN
	90MOR	20/3	393.0	583.1	3.2E+2	1.6E+5	0.03	note	99.94	sta	90MOR
	93JOS	33/18	303.4	467.3	2.8E-1	8.0E+3	0.02	2 %	98+	sta	88SAS/JOS
	54CAM/FOR	*16/0*	*463.2*	*559.9*	*6.9E+3*	*1.0E+5*	*0.002*	*5 Pa*	*99.97*	*dyn*	*45WIL/TAY*
heptadecane	49BRA/SHE	eqn.	298.1	313.1	6.1E-2	3.1E-1	nosp	nosp	nosp	wef	46BRA/EVA
	51TIL/PES	1/1	426.8		9.3E+2		nosp	nosp	nosp	nosp	
	81GRE/POT	5/4	357.8	434.0	1.5E+1	1.4E+3	0.1	nosp	nosp	sat	77GRE/BON
	93JOS	25/15	313.6	467.3	3.0E-1	5.0E+3	0.02	2 %	98+	sta	88SAS/JOS
octadecane	49BRA/SHE	eqn.	303.1	313.1	3.6E-2	1.1E-1	nosp	nosp	nosp	wef	46BRA/EVA
	51TIL/PES	1/1	426.4		5.3E+2		nosp	nosp	nosp	nosp	
	55MYE/FEN	26/8s	375.5	586.2	2.7E+1	1.0E+5	0.2	nosp	nosp	dyn	55MEY/FEN
	79MAC/PRA	10/10	318.1	361.2	2.2E-1	9.7E+0	nosp	2.2%	99+	sat	79MAC/PRA
	81GRE/POT	5/5	357.8	434.0	6.7E+0	7.5E+2	0.1	nosp	nosp	sat	77GRE/BON
	86ALL/JOS1	11/11	335.2	439.8	1.2E+0	1.0E+3	0.02	1 %	nosp	sat	86ALL/JOS1
	90MOR	17/3	413.0	588.1	2.7E+2	9.8E+4	0.03	note	99.8	sta	90MOR
	93JOS	17/12	323.5	453.0	3.3E-1	1.8E+3	0.02	2 %	98+	sta	88SAS/JOS
	93JOS	28/18	324.4	468.1	3.0E-1	3.1E+3	0.02	2 %	98+	sta	88SAS/JOS
nonadecane	51TIL/PES	1/1	442.1		6.7E+2		nosp	nosp	nosp	nosp	
	64MOR	3/3	306.1	328.1	1.9E-2	2.1E-1	0.02	nosp	nosp	wef	49BRA/SHE
	81GRE/POT	4/4	379.1	434.0	1.6E+1	4.2E+2	0.1	nosp	nosp	sat	77GRE/BON
	90MOR	16/3	423.0	588.1	2.6E+2	7.4E+4	0.03	note	99.2	sta	90MOR
	92KAS	10/8	373.8	459.2	1.4E+1	1.4E+3	0.02	2 %	98+	sta	88SAS/JOS
	93JOS	15/12	334.2	467.2	3.8E-1	1.9E+3	0.02	2 %	98+	sta	88SAS/JOS
eicosane	51TIL/PES	1/1	456.4		6.7E+2		nosp	nosp	nosp	nosp	
	55SCH/WHI	5/4s	410.1	469.6	6.7E+1	1.3E+3	0.5	nosp	nosp	dyn	55MEY/FEN
	55MYE/FEN	26/8s	395.0	615.2	2.7E+1	1.0E+5	0.2	nosp	nosp	dyn	55MEY/FEN
	79MAC/PRA	7/7	344.3	380.4	4.1E-1	9.1E+0	nosp	2.2%	99+	sat	79MAC/PRA
	81GRE/POT	5/5	357.8	434.0	1.2E+0	2.4E+2	0.1	nosp	nosp	sat	77GRE/BON
	88SAS/JOS	21/19	363.2	467.3	2.3E+0	1.3E+3	0.02	2 %	98+	sta	88SAS/JOS
	89CHI/NGU	13/9	388.1	488.1	1.6E+1	2.8E+3		<1 Pa	99.95	sta	66OSB/DOU
	90MOR	16/3	433.0	588.1	2.4E+2	5.4E+4	0.03	note	99.9	sta	90MOR
	91PIA/POM	8/8	315.0	366.0	2.9E-2	4.5E+0	0.5	nosp	99+	wef	90PIA/SCA
	91PIA/POM	59/59	339.5	393.0	3.8E-1	3.2E+1	nosp	nosp	99+	tef	91PIA/POM
	91PIA/POM	55/52	398.0	472.0	2.4E+1	1.2E+3	nosp	nosp	99+	sat	91PIA/POM
	93JOS	15/14	342.3	467.2	4.0E-1	1.2E+3	0.02	2 %	98+	sta	88SAS/JOS
	89CHI/NGU	*16/0*	*523.9*	*626.0*	*9.6E+3*	*1.2E+5*		*<5 Pa*	*99.95*	*dyn*	*66OSB/DOU*

Note: pressure error for Morgan's data (90MOR) can be estimated from the equation $\sigma p = 0.00015p + 4.7988$ where pressure is in Pa.

TABLE 3. Vapor pressures included in the simultaneous correlation, the selected medium pressure source (all p_{sat} > 1 kPa) is listed in italics

Alkane	Reference	No. pts.	T_{min}	T_{max}	p_{min}	p_{max}	σ_{min}	σ_{max}	d_w	d	d_r	d_b	+/−
			K		Pa		Pa			Pa	%	Pa	
pentane	*74OSB/DOU*	*10*	*268.8*	*314.5*	*2.0E+4*	*1.2E+5*	*5.1*	*6.2*	*0.48*	*2.7*	*0.01*	*−0.4*	*−2*
hexane	*45WIL/TAY*	*15*	*286.2*	*342.7*	*1.2E+4*	*1.0E+5*	*5.1*	*8.3*	*0.55*	*3.5*	*0.01*	*0.5*	*−1*
heptane	*49FOR/NOR*	*20*	*299.2*	*372.4*	*6.4E+3*	*1.0E+5*	*7.1*	*11.0*	*0.58*	*4.9*	*0.03*	*1.0*	*2*
octane	*45WIL/TAY*	*29*	*326.0*	*399.7*	*7.7E+3*	*1.0E+5*	*4.0*	*20.0*	*0.68*	*7.1*	*0.03*	*0.6*	*3*
nonane	*49FOR/NOR*	*20*	*343.5*	*424.9*	*6.4E+3*	*1.0E+5*	*5.0*	*7.4*	*0.93*	*5.4*	*0.03*	*−0.5*	*−6*
decane	89CHI/NGU	12	268.1	348.1	1.7E+1	3.2E+3	0.2	0.4	0.95	0.3	0.33	0.0	6
	89CHI/NGU	*16*	*373.2*	*454.3*	*9.6E+3*	*1.2E+5*	*0.6*	*3.8*	*1.06*	*1.6*	*0.01*	*−0.2*	*2*
undecane	92KAS	9	293.4	373.2	4.1E+1	4.4E+3	0.8	44.0	1.29	13.6	2.30	10.9	9
	93JOS	17	293.8	382.1	4.1E+1	6.4E+3	0.8	64.0	0.41	4.6	0.77	0.1	−1
	55CAM/ROS	*18*	*384.1*	*470.4*	*7.0E+3*	*1.0E+5*	*5.0*	*7.1*	*0.84*	*5.1*	*0.02*	*0.0*	*−2*
dodecane	86ALL/JOS1	15	313.2	389.6	5.8E+1	4.3E+3	4.3	25.3	0.49	3.5	1.00	1.8	11
	86ALL/JOS2	4	313.4	352.0	6.0E+1	6.9E+2	1.2	14.0	0.32	1.4	0.64	1.0	2
	88SAS/JOS	21	313.4	371.2	5.9E+1	1.8E+3	1.2	19.0	0.43	5.0	0.64	−2.8	−5
	92KAS	9	313.4	403.2	6.2E+1	7.3E+3	1.2	73.0	1.29	40.5	2.02	−17.8	3
	93JOS	16	313.4	402.1	6.2E+1	7.0E+3	1.2	71.0	0.60	9.2	1.02	−5.9	−6
	45WIL/TAY	*17*	*408.4*	*490.5*	*9.0E+3*	*1.0E+5*	*5.0*	*6.9*	*0.85*	*5.5*	*0.01*	*0.1*	*5*
tridecane	93JOS	14	323.7	402.3	4.7E+1	3.7E+3	0.9	40.0	0.42	5.1	0.72	2.3	4
	55CAM/ROS	*14*	*412.4*	*509.2*	*5.5E+3*	*1.0E+5*	*7.0*	*40.0*	*0.59*	*9.0*	*0.04*	*2.4*	*2*
tetradecane	86ALL/JOS1	6	343.1	394.7	7.2E+1	1.3E+3	7.0	13.0	0.27	2.7	1.49	−0.7	0
	93JOS	18	344.0	422.2	7.6E+1	4.4E+3	1.5	44.0	0.39	5.3	0.56	2.1	10
	55CAM/ROS	*10*	*439.1*	*527.3*	*8.3E+3*	*1.0E+5*	*8.0*	*40.0*	*0.66*	*15.5*	*0.03*	*3.0*	*2*
pentadecane	86ALL/JOS1	5	346.0	409.1	3.6E+1	1.3E+3	2.8	9.4	0.59	4.9	0.84	−2.8	−3
	93JOS	10	343.8	432.4	3.1E+1	3.7E+3	0.6	37.0	0.30	2.5	0.58	−1.3	−2
	55CAM/ROS	*10*	*442.8*	*543.7*	*5.5E+3*	*1.0E+5*	*7.0*	*40.0*	*0.84*	*10.2*	*0.07*	*3.6*	*4*
hexadecane	93JOS	19	363.9	452.3	5.5E+1	4.7E+3	1.1	46.0	0.40	7.1	0.61	4.9	15
	54CAM/FOR	*16*	*463.2*	*559.9*	*6.9E+3*	*1.0E+5*	*5.0*	*30.0*	*0.89*	*10.7*	*0.04*	*2.4*	*0*
heptadecane	interpol	21	302.4	575.4	1.0E−1	1.0E+5	0.0	62.0	0.14	5.6	0.15	0.7	3
octadecane	interpol	21	312.0	590.0	1.0E−1	1.0E+5	0.0	62.0	0.24	10.3	0.24	1.4	−3
nonadecane	interpol	21	321.1	604.0	1.0E−1	1.0E+5	0.0	99.0	0.32	16.4	0.42	2.0	−9
eicosane	79MAC/PRA	7	344.3	380.4	4.1E−1	9.1E+0	0.0	0.2	1.31	0.1	2.59	0.1	−1
	89CHI/NGU	13	388.1	488.1	1.6E+1	2.8E+3	0.2	0.6	2.32	1.0	0.34	−0.2	3
	89CHI/NGU	*12*	*523.9*	*591.3*	*9.6E+3*	*5.8E+4*	*0.5*	*2.6*	*1.94*	*3.3*	*0.01*	*0.0*	*2*

All values for C_{17} to C_{19} *n*-alkanes were obtained by interpolation; no experimental data were considered.

TABLE 4. Rejected vapor pressures

Alkane	Reference	d Pa	d_r %	d_b Pa	+/−
pentane	40MES/KEN	5.7	1.41	5.7	1
	51TIC/LOS	24.5	20.42	−14.2	−12
	73CAR/KOB	29.2	12.28	−16.2	−6
	75HOR/HOP	11.1	1.39	10.9	2
hexane	64WOL/HOP	38.2	8.40	38.2	1
	65WOL/HOP	43.6	9.82	36.1	3
	66WOL/HOP	75.4	33.93	72.4	2
	68WOL/WUR	39.1	15.32	39.1	2
	73CAR/KOB	9.2	11.30	−4.9	1
heptane	73CAR/KOB	8.1	8.15	−4.8	1
octane	31LIN	9.3	2.04	−7.3	−3
	58COO	29.1	7.48	−29.1	−1
	73CAR/KOB	10.1	7.91	−5.5	−4
nonane	64WOL/HOP	22.7	30.23	20.4	3
	73CAR/KOB	102.4	28.11	−44.1	−4
	79SCH/RAL	53.8	7.20	53.8	1
decane	31LIN	5.4	14.06	4.4	4
	73CAR/KOB	81.5	24.03	−40.4	−4
	86ALL/JOS1	4.6	0.94	−4.2	−6
	90MOR	2.0	0.23	−2.0	−1
	93JOS	0.6	1.84	0.4	10
dodecane	51TIL/PES	100.1	12.20	−100.1	−1
	90MOR	4.9	0.16	3.2	1
tridecane	51TIL/PES	23.3	6.19	23.3	1
tetradecane	31LIN	1.0	99.06	−1.0	−1
	51TIL/PES	30.6	4.82	30.6	1
	90MOR	428.6	0.29	44.1	−2
hexadecane	49BRA/SHE	0.0	13.34	0.0	4
	49PAR/MOO	0.0	4.78	0.0	0
	51TIL/PES	68.3	14.58	−68.3	−1
	55MYE/FEN	17.1	3.24	−11.4	−8
	69EGG/SEI	19.6	3.90	−5.2	6
	81GRE/POT	18.0	4.70	9.2	1
	87MIL/FEN	6.6	0.86	−4.1	0
	90MOR	7.6	1.18	6.9	3
heptadecane	49BRA/SHE	0.0	2.33	0.0	−4
	51TIL/PES	3.0	0.33	3.0	1
	81GRE/POT	37.7	5.56	19.0	1
	93JOS	16.4	2.72	9.4	21
octadecane	49BRA/SHE	0.0	1.30	0.0	−3
	51TIL/PES	18.5	3.59	18.5	1
	55MYE/FEN	20.6	4.57	16.2	8
	79MAC/PRA	0.2	7.92	0.2	10
	81GRE/POT	2.2	4.27	0.0	−1
	86ALL/JOS1	7.4	4.70	2.6	3
	90MOR	246.0	1.23	106.2	17
	93JOS	28.6	3.98	18.4	15
	93JOS	47.5	5.39	−31.6	−28
nonadecane	51TIL/PES	29.0	4.55	29.0	1
	64MOR	0.0	2.92	0.0	−1
	81GRE/POT	7.8	2.93	−4.5	−4
	90MOR	389.3	2.85	154.7	16
	92KAS	7.7	10.68	5.7	8
	93JOS	11.2	3.30	6.4	13
eicosane	51TIL/PES	79.7	10.68	−79.7	−1
	55SCH/WHI	4.1	1.70	−3.0	−2
	55MYE/FEN	19.2	4.18	−9.7	2
	81GRE/POT	3.7	8.41	−1.7	−3
	88SAS/JOS	9.5	3.26	5.2	19
	90MOR	5.0	1.71	4.6	3
	91PIA/POM	0.7	76.21	0.4	8
	91PIA/POM	3.3	33.84	2.2	59
	91PIA/POM	149.0	22.53	−101.3	−38
	93JOS	2.5	6.29	−0.5	8

TABLE 5. Enthalpies of vaporization included in the simultaneous correlation

Alkane	Reference	No. pts.	T_{min} K	T_{max}	p_{min} Pa	p_{max}	σ_r %	d_w	d kJ·mol^{-1}	d_r %	d_b kJ·mol^{-1}	+/−
pentane	81HOS/SCO	5	259.6	298.2	1.3E+4	6.8E+4	0.2	0.31	0.02	0.06	0.02	5
	47OSB/GIN	1	298.2		6.8E+4		0.1	0.02	0.00	0.00	0.00	1
hexane	47OSB/GIN	1	298.2		2.0E+4		0.1	1.00	0.03	0.10	0.03	1
	79MAJ/SVO	2	298.2	313.2	2.0E+4	3.7E+4	0.3	0.33	0.03	0.10	0.03	2
	47WAD/DOU	1	308.8		3.1E+4		0.2	0.39	0.02	0.08	0.02	1
heptane	47OSB/GIN	1	298.2		6.1E+3		0.1	0.44	0.02	0.04	−0.02	−1
	79MAJ/SVO	3	298.2	333.2	6.1E+3	2.8E+4	0.3	0.15	0.02	0.04	0.02	3
	47WAD/DOU	1	331.3		2.6E+4		0.2	0.45	0.03	0.09	0.03	1
octane	47OSB/GIN	1	298.2		1.9E+3		0.1	1.78	0.07	0.18	−0.07	−1
	66WAD	1	298.2		1.9E+3		0.5	0.26	0.05	0.13	−0.05	−1
	79MAJ/SVO	4	298.2	353.2	1.9E+3	2.3E+4	0.3	0.44	0.05	0.13	−0.04	−2
	81HOS/SCO	4	337.6	366.9	1.3E+4	3.8E+4	0.2	0.22	0.02	0.04	0.01	2
nonane	47OSB/GIN	1	298.2		5.8E+2		0.1	2.52	0.12	0.25	−0.12	−1
	84MAJ/SVO	4	328.2	368.2	3.1E+3	1.8E+4	0.3	0.14	0.02	0.04	−0.02	−4
decane	47OSB/GIN	1	298.1		1.8E+2		0.1	1.14	0.06	0.11	−0.06	−1
	66WAD	1	298.1		1.8E+2		0.5	0.31	0.08	0.15	−0.08	−1
	71MOR	1	298.1		1.8E+2		0.5	0.31	0.08	0.15	−0.08	−1
	73SAI/KUS	1	298.1		1.8E+2		0.5	0.35	0.09	0.17	−0.09	−1
	63COU/KOZ	4	344.3	394.3	2.7E+3	2.1E+4	2.0	0.24	0.21	0.47	−0.17	−4
undecane	66WAD	1	298.2		5.7E+1		0.5	0.50	0.14	0.25	−0.14	−1
dodecane	72MOR	1	298.2		1.8E+1		1.0	0.38	0.23	0.37	−0.23	−1
	76MEL/MAN	1	298.2		1.8E+1		1.0	0.42	0.26	0.42	0.26	1
	81SHI	1	298.2		1.8E+1		1.0	0.41	0.25	0.41	−0.25	−1
tridecane	72MOR	1	298.2		5.7E+0		2.0	0.24	0.31	0.47	−0.31	−1
	79SUN/SVE	6	308.2	348.2	1.4E+1	2.3E+2	2.0	0.13	0.16	0.25	0.07	2
tetradecane	72MOR	1	298.2		1.8E+0		2.0	0.44	0.63	0.88	−0.63	−1
	79SUN/SVE	7	313.2	358.2	7.1E+0	1.9E+2	2.0	0.38	0.51	0.76	0.33	3
pentadecane	72MOR	1	298.2		5.8E−1		2.0	0.38	0.58	0.75	−0.58	−1
	79SUN/SVE	6	333.2	373.2	1.4E+1	2.1E+2	2.0	0.49	0.68	0.99	0.38	2
hexadecane	72MOR	1	298.2		1.9E−1		2.0	0.02	0.03	0.04	0.03	1
heptadecane	[a]72MOR	1	298.2		6.2E−2		3.0	0.17	0.44	0.51	−0.44	−1

[a] ΔH_{vap} for heptadecane was not considered in the final simultaneous correlation.

TABLE 6. Parameters of Equation (29) for calculating ideal gas heat capacities

Alkane	A	B_1	C_1	B_2	C_2
pentane	86.389058	163.62772	1404.5312	125.55904	3247.1465
hexane	101.85997	196.40919	1400.5301	137.69426	3214.2702
heptane	117.22475	151.73507	3154.9913	227.31996	1391.9171
octane	132.49098	166.06550	3048.8270	254.85474	1378.6073
nonane	148.15036	288.24904	1380.8003	178.57491	3051.1566
decane	163.73837	320.24325	1379.9706	191.23849	3024.7636
undecane	179.21063	350.72479	1376.4867	205.11522	2988.5224
dodecane	194.67625	219.19909	2956.5645	381.04958	1373.3800
tridecane	210.13549	411.22701	1370.5730	233.46990	2928.1171
tetradecane	225.58955	247.90156	2902.6832	441.27841	1368.0279
pentadecane	241.04038	262.46130	2879.9394	471.23544	1365.7312
hexadecane	256.48610	277.15855	2859.2830	501.07642	1363.6061
heptadecane	271.92811	291.96985	2840.5163	530.82470	1361.6474
octadecane	287.36648	306.88739	2823.3681	560.48430	1359.8298
nonadecane	302.80205	321.89530	2807.6748	590.07027	1358.1451
eicosane	318.23450	336.99194	2793.2187	619.58058	1356.5700

Parameters are valid in the temperature range between 200 and 1000 K.

TABLE 7. Review of heat capacity differences ΔC°_{vap} considered for inclusion in the simultaneous correlation

Alkane	No. pts.	T_{min}	T_{max}	p_{min}	p_{max}	σ_{min}	σ_{max}	d_w	d	d_r	d_b	+/−
		K		Pa		$J\cdot K^{-1}\cdot mol^{-1}$			$J\cdot K^{-1}\cdot mol^{-1}$	%	$J\cdot K^{-1}\cdot mol^{-1}$	
pentane	23	148.6	258.6	2.1E−1	1.2E+4	1.7	2.4	0.42	0.41	0.79	0.03	5
hexane	23	180.4	290.4	1.7E+0	1.4E+4	1.8	3.2	0.42	0.50	0.85	0.03	3
heptane	27	182.6	312.6	1.7E−1	1.2E+4	1.6	3.0	1.61	2.18	3.23	0.68	15
octane	23	222.6	332.6	4.2E+0	1.0E+4	2.0	3.8	0.66	1.14	1.56	0.13	9
nonane	19	225.0	315.0	8.5E−1	1.6E+3	2.0	4.4	1.50	2.86	3.47	−0.43	5
decane	27	247.0	377.0	2.1E+0	1.1E+4	2.3	4.6	1.41	3.11	3.66	−1.78	−13
undecane	31	251.7	401.7	7.1E−1	1.4E+4	2.3	6.8	0.93	3.01	3.51	1.40	19
dodecane	12	266.7	321.7	8.9E−1	1.1E+2	2.5	4.5	0.99	2.80	2.78	−0.39	2
tridecane	7	271.7	301.7	3.9E−1	7.8E+0	2.5	3.1	0.94	2.87	2.59	−0.15	1
tetradecane	4	282.8	297.8	3.7E−1	1.7E+0	3.1	3.4	0.57	2.18	1.85	−0.37	0
pentadecane	6	285.5	310.5	1.4E−1	2.0E+0	2.7	3.2	0.82	2.98	2.39	−0.03	0
hexadecane	10	293.2	338.2	1.1E−1	8.3E+0	2.8	3.7	0.90	3.60	2.86	−0.30	2
heptadecane [a]	17	301.9	381.9	9.5E−2	8.2E+1	3.0	4.5	1.36	6.55	5.26	5.19	11
octadecane [a]	16	301.3	376.3	2.9E−2	2.8E+1	3.0	4.5	1.45	7.32	5.49	5.44	10
nonadecane [a]	30	305.2	450.2	1.6E−2	9.3E+2	5.0	8.8	1.11	9.71	7.53	9.26	30
eicosane [a]	16	325.0	400.0	5.8E−2	3.5E+1	20.8	24.1	0.24	8.97	6.24	−7.23	−14

[a] ΔC°_{vap} values for C_{17} to C_{20} *n*-alkanes were not considered in the final simultaneous correlation.

TABLE 8. Critical parameters and acentric factors for *n*-alkanes (92DIP)

Alkane	T_c K	p_c MPa	ω
pentane	469.7	3.370	0.251
hexane	507.6	3.025	0.299
heptane	540.2	2.74	0.350
octane	568.7	2.49	0.397
nonane	594.6	2.29	0.443
decane	617.7	2.11	0.490
undecane	639	1.98	0.533
dodecane	658	1.82	0.573
tridecane	675	1.68	0.618
tetradecane	693	1.57	0.654
pentadecane	708	1.48	0.696
hexadecane	723	1.40	0.737
heptadecane	736	1.34	0.772
octadecane	747	1.29	0.812
nonadecane	758	1.23	0.844
eicosane	769	1.16	0.891

TABLE 9. Differences between temperatures resulting from isobaric plots (Eq. 34) and those obtained from the Cox equation (19)

The corresponding pressure differences are given in parentheses (in per cent up to 1000 Pa and in Pa at the two higher pressures)

p_{sat}/Pa	0.1		1		10		100		1000		10 000		101 325	
	δT (δp)													
	K	(%)	K	(%)	K	(%)	K	(%)	K	(%)	K	(Pa)	K	(Pa)
pentane	0.16	(−3.1)	0.15	(−2.3)	0.09	(−1.1)	0.13	(−1.2)	0.00	(0.0)	0.01	(− 1)	0.00	(−3)
hexane	−0.04	(0.6)	−0.05	(0.8)	−0.05	(0.6)	−0.07	(0.7)	0.01	(−0.1)	0.00	(2)	0.00	(10)
heptane	−0.30	(5.2)	−0.27	(3.9)	−0.19	(2.2)	−0.19	(1.7)	−0.02	(0.2)	0.00	(3)	0.01	(−15)
octane	−0.09	(1.5)	−0.10	(1.3)	−0.04	(0.4)	−0.10	(0.9)	0.01	(0.1)	0.00	(0)	0.00	(11)
nonane	−0.07	(1.0)	−0.07	(0.8)	0.01	(−0.1)	−0.06	(0.4)	−0.01	(0.0)	0.02	(−5)	0.00	(8)
decane	0.27	(−3.7)	0.21	(−2.3)	0.19	(−1.8)	0.05	(−0.4)	0.01	(0.0)	0.00	(1)	0.00	(−3)
undecane	−0.05	(0.7)	−0.05	(0.5)	0.02	(−0.2)	−0.02	(0.1)	−0.01	(0.1)	0.01	(−1)	0.00	(−3)
dodecane	0.04	(−0.5)	0.02	(−0.3)	0.06	(−0.5)	0.01	(−0.1)	0.00	(0.0)	0.01	(−2)	0.00	(0)
tridecane	−0.12	(1.6)	−0.09	(1.0)	−0.03	(0.3)	−0.04	(0.3)	0.00	(0.0)	0.00	(0)	0.01	(−19)
tetradecane	−0.17	(2.0)	−0.14	(1.4)	−0.09	(0.7)	−0.07	(0.5)	−0.01	(0.1)	0.00	(0)	0.00	(10)
pentadecane	−0.19	(2.3)	−0.17	(1.7)	−0.13	(1.1)	−0.11	(0.7)	−0.02	(0.1)	0.01	(0)	−0.02	(34)
hexadecane	0.10	(−1.2)	0.06	(−0.6)	0.01	(−0.1)	−0.03	(0.2)	0.02	(−0.1)	0.00	(1)	0.00	(−13)
eicosane	0.06	(−0.2)	0.02	(−0.2)	0.02	(−0.1)	0.00	(−0.1)	0.00	(0.0)	0.01	(0)	−0.08	(183)

TABLE 10. Recommended vapor pressures, parameters of the Cox Eq. (19)

Alkane	Parameters				
	A_0	A_1	A_2	T_0/K	p_0/kPa
pentane	2.73425	−1.966544E-3	2.408406E-6	309.209	101.325
hexane	2.79797	−2.022083E-3	2.287564E-6	341.863	101.325
heptane	2.86470	−2.113204E-3	2.250991E-6	371.552	101.325
octane	2.90150	−2.046204E-3	2.010759E-6	398.793	101.325
nonane	2.94690	−2.051933E-3	1.903683E-6	423.932	101.325
decane	2.96690	−1.932579E-3	1.644626E-6	447.269	101.325
undecane	3.02711	−2.045579E-3	1.712658E-6	469.042	101.325
dodecane	3.05854	−2.018454E-3	1.606849E-6	489.438	101.325
tridecane	3.10403	−2.071819E-3	1.611600E-6	508.602	101.325
tetradecane	3.13624	−2.063853E-3	1.541507E-6	526.691	101.325
pentadecane	3.16774	−2.062348E-3	1.487263E-6	543.797	101.325
hexadecane	3.18271	−2.002545E-3	1.384476E-6	559.978	101.325
heptadecane	3.21826	−2.036553E-3	1.383899E-6	575.375	101.325
octadecane	3.24741	−2.048039E-3	1.362445E-6	590.023	101.325
nonadecane	3.27626	−2.062714E-3	1.346737E-6	603.989	101.325
eicosane	3.31181	−2.102218E-3	1.348780E-6	617.415	101.325

TABLE 11. Statistical characteristics of the final correlation

Alkane	s_w	p_{sat}	d_w ΔH_{vap}	ΔC°_{vap}	K_H	K_C	d/Pa sim.c.	(mpr) p_{sat}only
pentane	0.44	0.48	0.29	0.42	1.000	1.000	2.7	2.3
hexane	0.51	0.55	0.60	0.42	1.000	1.000	3.5	3.3
heptane	1.26	0.58	0.31	1.61	1.000	1.000	4.9	2.8
octane	0.68	0.68	0.65	0.66	1.000	1.000	7.1	6.8
nonane	1.27	0.93	1.14	1.50	1.414	1.100	5.4	2.8
decane	1.19	1.01	0.48	1.41	1.000	1.000	1.6	1.1
undecane	0.89	0.84	0.50	0.93	1.000	1.000	5.1	4.8
dodecane	0.75	0.71	0.40	0.99	1.000	1.000	5.5	5.4
tridecane	0.59	0.51	0.15	0.94	1.000	1.000	9.5	9.0
tetradecane	0.48	0.47	0.39	0.57	1.000	1.000	16.0	15.5
pentadecane	0.66	0.62	0.47	0.82	1.000	1.000	10.2	7.6
hexadecane	0.74	0.67	0.02	0.90	1.000	1.000	10.7	9.7
heptadecane	0.15	0.14	0.17[a]	1.36[a]	0.000	0.000		
octadecane	0.26	0.24		1.45[a]	0.000	0.000		
nonadecane	0.34	0.32		1.11[a]	0.000	0.000		
eicosane	2.09	1.99		0.24[a]	0.000	0.000	3.3	1.0

[a]Thermal data were not included in the correlation for C_{17} to C_{20} *n*-alkanes

TABLE 12. Recommended vapor pressures, temperatures T/K at selected p_{sat} values calculated from the Cox equation

Alkane	p_{sat}/Pa						
	0.1	1	10	100	1000	10 000	101 325
pentane	144.82	157.65	173.37	193.17	219.13	255.05	309.21
hexane	162.64[h]	176.70[h]	193.88	215.51	243.81	282.95	341.86
heptane	179.40[h]	194.52	212.98	236.18	266.53	308.48	371.55
octane	194.67[h]	210.84[h]	230.53	255.25	287.52	332.03	398.79
nonane	209.23[h]	226.30	247.08	273.13	307.09	353.86	423.93
decane	222.67[h]	240.65[h]	262.50	289.84	325.40	374.25	447.27
undecane	236.04[h]	254.71	277.39	305.75	342.64	393.33	469.04
dodecane	248.34[h]	267.74	291.28	320.68	358.87	411.27	489.44
tridecane	260.30[h]	280.31	304.58	334.89	374.24	428.21	508.60
tetradecane	271.60[h]	292.22	317.21	348.38	388.82	444.22	526.69
pentadecane	282.39[h]	303.58	329.24	361.22	402.67	459.40	543.80
hexadecane	292.41	314.20	340.55	373.36	415.82	473.84	559.98
heptadecane	302.38	324.64	351.56	385.06	428.40	487.59	575.38[e]
octadecane	311.88	334.61	362.08	396.24	440.41	500.70	590.02[e]
nonadecane	321.02	344.18	372.17	406.95	451.91	513.24	603.99[e]
eicosane	330.01	353.55	381.97	417.30	462.95	525.23	617.41[e]

[h]Hypothetical values below the triple point temperature.
[e]Values obtained by extrapolation; probable decomposition at this temperature.

TABLE 13. Recommended enthalpies of vaporization; ΔH_{vap} in kJ·mol^{-1} at selected values of p_{sat}

Alkane	p_{sat}/Pa						
	0.1	1	10	100	1000	10 000	101 325
pentane	34.38	33.70	32.87	31.83	30.50	28.68	25.82 (25.79)
hexane	39.56[h]	38.68[h]	37.62	36.31	34.64	32.39	28.95 (28.85)
heptane	44.72[h]	43.61	42.28	40.66	38.61	35.91	31.87 (31.77)
octane	49.24[h]	47.98[h]	46.46	44.62	42.30	39.24	34.61 (34.41)
nonane	53.82[h]	52.36	50.62	48.50	45.87	42.40	37.18
decane	57.83[h]	56.25[h]	54.38	52.10	49.24	45.45	39.58 (38.75)
undecane	62.56[h]	60.71	58.52	55.88	52.62	48.35	41.91
dodecane	66.62[h]	64.60	62.21	59.34	55.79	51.14	44.09
tridecane	70.91[h]	68.65	65.98	62.80	58.89	53.82	46.20
tetradecane	74.88[h]	72.42	69.54	66.10	61.89	56.42	48.16
pentadecane	78.75[h]	76.10	72.99	69.29	64.78	58.92	50.08
hexadecane	82.09	79.32	76.07	72.20	67.48	61.31	51.84
heptadecane	85.89	82.89	79.38	75.23	70.18	63.62	53.58[e]
octadecane	89.47	86.27	82.54	78.13	72.79	65.85	55.23[e]
nonadecane	92.98	89.57	85.62	80.95	75.32	68.04	56.93[e]
eicosane	96.69	93.03	88.80	83.83	77.84	70.14	58.49[e]

[h]Hypothetical values below the triple point temperature.
[e]Values obtained by extrapolation; probable decomposition at this temperature, recommended values based on calorimetric measurements (85MAJ/SVO) are given in parentheses.

TABLE 14. Recommended values of p_{sat}, ΔH_{vap} and ΔC°_{vap} at the triple point temperature

Alkane	T K	p_{sat} Pa	ΔH_{vap} kJ·mol^{-1}	ΔC°_{vap} J·K^{-1}·mol^{-1}
pentane	143.48	0.077	34.45	−52.68
hexane	177.87	1.189	38.61	−62.03
heptane	182.59	0.169	44.48	−73.16
octane	216.41	2.018	47.54	−77.13
nonane	219.69	0.431	52.92	−85.30
decane	243.52	1.393	56.01	−86.54
undecane	247.60	0.437	61.41	−98.70
dodecane	263.59	0.632	65.03	−103.56
tridecane	267.78	0.249	70.06	−113.40
tetradecane	279.02	0.240	73.99	−119.48
pentadecane	283.09	0.109	78.66	−126.63
hexadecane	291.32	0.088	82.23	−129.01
heptadecane	295.13	0.043	86.88	−137.72
octadecane	301.32	0.030	90.99	−144.61
nonadecane	305.08	0.016	95.38	−152.05
eicosane	309.68	0.010	99.94	−161.74

TABLE 15. Recommended values at 298.15 K

Alkane	p_{sat} Pa	ΔH_{vap} kJ·mol^{-1}	$\Delta H'$ kJ·mol^{-1}	ΔC°_{vap} J·K^{-1}·mol^{-1}	$\Delta C'$ J·K^{-1}·mol^{-1}
pentane	6.835E+4	26.42	27.44	−45.84	−29.39
hexane	2.018E+4	31.52	32.07	−52.63	−41.88
heptane	6.102E+3	36.57	36.86	−60.94	−54.21
octane	1.872E+3	41.56	41.71	−67.69	−63.65
nonane	5.807E+2	46.55	46.63	−75.67	−73.35
decane	1.820E+2	51.42	51.46	−80.56	−79.26
undecane	5.689E+1	56.58	56.59	−91.77	−91.07
dodecane	1.802E+1	61.52	61.53	−98.80	−98.43
tridecane	5.682E+0	66.68	66.68	−108.81	−108.62
tetradecane	1.804E+0	71.73	71.73	−116.57	−116.48
pentadecane	5.760E−1	76.77	76.77	−124.37	−124.32
hexadecane	1.910E−1	81.35	81.35	−128.08	−128.06
heptadecane	6.148E−2	86.47	86.47	−137.28	−137.27
octadecane[h]	2.007E−2	91.44	91.44	−145.10	−145.09
nonadecane[h]	6.573E−3	96.44	96.44	−153.13	−153.13
eicosane[h]	2.091E−3	101.81	101.81	−163.66	−163.66

[h]Hypothetical values below the triple point temperature.

TABLE 16. Differences of p_{sat} in major secondary sources from the recommended vapor pressures 0.1, 1, 10 and 100 Pa

Vapor pressures used for determining δp_{sat} (%) relate to the temperatures listed in Table 12.

	δp_{sat} / %																			
	KING[a]				89AMB/WAL				87TRC[b]				89DAU/DAN[c]				92DIP[d]			
p_{sat}/Pa	0.1	1	10	100	0.1	1	10	100	0.1	1	10	100	0.1	1	10	100	0.1	1	10	100
C_5					−7.0	−4.2	−2.1	−0.7	9.7	6.3	2.4	−0.6	−29.5	−23.1	−17.0	−11.3	−8.9	−5.9	−3.5	−1.7
C_6	−3.5	−1.4	−0.1	0.3	−2.5	−1.1	−0.2	0.2	−60.2	−3 9.3	−20.1	−6.7	−46.2	−33.2	−20.5	−9.6	−33.3	−24.4	−15.9	−8.5
C_7	2.7	2.7	2.2	1.3	3.1	2.7	2.1	1.3	−40.0	−23.8	−11.5	−4.1	−28.5	−19.8	−12.1	−6.0	9.4	6.2	3.4	1.2
C_8	1.9	2.0	1.6	1.0	2.1	2.0	1.6	1.0	73.9	39.7	16.9	3.4	49.0	31.0	17.2	7.2	7.9	5.6	3.4	1.5
C_9	4.1	3.5	2.4	1.3	4.7	3.6	2.4	1.3	89.6	47.3	20.1	4.4	61.1	37.0	19.6	7.8	0.2	0.3	0.2	0.0
C_{10}	0.7	1.3	1.4	1.0	1.2	1.4	1.3	0.9	85.0	44.3	18.2	3.3	64.7	38.5	19.7	6.9	0.3	0.2	−0.1	−0.4
C_{11}	2.0	1.7	1.1	0.4	6.9	5.0	3.2	1.7					−18.5	−11.9	−6.5	−2.7	−7.8	−5.4	−3.4	−1.9
C_{12}	7.0	5.4	3.6	2.0	7.5	5.4	3.5	1.9	−3.6	−0.3	0.1	−0.8	12.2	5.8	1.4	−1.0	−3.8	−2.2	−1.1	−0.4
C_{13}	3.5	2.3	1.2	0.2	9.1	6.3	3.9	2.0	−0.4	0.7	−0.4	−1.9	61.1	42.6	27.6	15.9	1.6	0.7	0.0	−0.6
C_{14}	11.9	8.7	5.6	2.9	12.1	8.5	5.3	2.8	3.9	4.0	1.9	−0.5	−24.7	−16.5	−9.4	−4.1	6.5	4.1	2.1	0.6
C_{15}	5.4	4.0	2.6	1.3	12.3	8.5	5.2	2.6	63.2	35.1	15.2	3.0	−27.7	−18.4	−10.4	−4.2	19.2	12.1	6.5	2.4
C_{16}	8.5	6.2	4.0	2.1	8.4	6.0	3.8	1.9	17.4	11.2	4.7	−0.1	−0.6	1.2	1.9	1.6	4.6	3.3	2.1	1.0
C_{17}					18.9	14.2	10.1	6.7	−54.0	−31.8	−12.8	−0.9	−47.4	−31.3	−15.5	−2.7	6.9	3.6	0.8	−1.2
C_{18}					26.0	20.0	14.8	10.5	−75.3	−49.8	−21.5	−0.7	11.2	7.4	5.0	3.8	12.0	7.2	3.4	0.8
C19					22.3	17.0	12.5	9.0	8.4	12.8	12.7	10.2	18.8	16.1	13.3	10.6	0.7	0.3	0.0	−0.1
C20					9.0	5.5	2.9	1.2	34.4	13.5	−0.7	−8.3	12.3	2.3	−4.2	−7.3	−0.8	−0.5	−0.5	−0.7

[a]Data for C_6 to C_{10}, C_{12}, C_{14}, C_{16} *n*-alkanes (74KIN/ALN); data for C_5, C_{11}, C_{13} and C_{15} *n*-alkanes (86KIN/MAH).
[b]TRC tables (87TRC), data sheet from June 30, 1974 (related to API44 data project).
[c]Identical with DIPPR tables 801 from 1988.
[d]DIPPR tables 801 from 1992.

TABLE 17. Differences of p_{sat} in major secondary sources from the recommended vapor pressures at 1, 10 and 101.325 kPa

Vapor pressures used for determining δp_{sat} (%) relate to the temperatures listed in Table 12.

	δp_{sat} / Pa														
	KING[a]			89AMB/WAL			87TRC44[b]			89DAU/DAN[c]			92DIP[d]		
p_{sat}/kPa	1	10	101.325	1	10	101.325	1	10	101.325	1	10	101.325	1	10	101.325
C_5				0	3	−3	−10	−2	12	−62	−210	489	−6	−5	41
C_6	2	−0	−32	2	5	−3	−7	10	−18	−20	92	−657	−28	12	−67
C_7	4	−5	2	5	−0	23	−8	−5	8	−19	−24	−438	−2	−55	−9
C_8	3	−7	30	4	−2	18	−9	−6	4	11	−111	336	1	−33	−130
C_9	3	−7	66	4	−6	−4	−8	−3	−1	9	−109	585	0	4	340
C_{10}	4	3	90	4	2	18	−13	−1	5	−2	−204	1376	−7	−86	−488
C_{11}	−1	−10	187	5	−1	14		−8	9	−5	7	−109	−7	−15	−109
C_{12}	7	7	117	6	2	1	−7	1	13	−14	−36	466	0	−6	−191
C_{13}	−3	−17	106	6	−2	20	−17	−33	69	74	226	661	−7	−34	371
C_{14}	10	14	149	10	6	−71	−9	−1	9	−9	15	64	−2	−30	155
C_{15}	4	10	32	8	1	28	−9	3	4	−5	62	492	−1	−72	322
C_{16}	7	14	149	6	−2	81	−13	−4	7	5	−51	−381	2	−6	137
C_{17}				42	252	1868	33	251	530	41	375	−1195	−22	−208	−625
C_{18}				71	487	3810	67	464	1231	35	320	744	−5	−34	1277
C19				63	464	3594	79	551	2073	78	512	2245	0	41	1552
C20				4	54	1283	−80	−303	1089	−70	−354	1005	−10	−108	342

[a]Data for C_6 to C_{10}, C_{12}, C_{14}, C_{16} *n*-alkanes (74KIN/ALN); data for C_5, C_{11}, C_{13} and C_{15} *n*-alkanes (86KIN/MAH).
[b]TRC tables (87TRC), data sheet from June 30, 1974 (related to API44 data project).
[c]Identical with DIPPR tables 801 from 1988.
[d]DIPPR tables 801 from 1992.

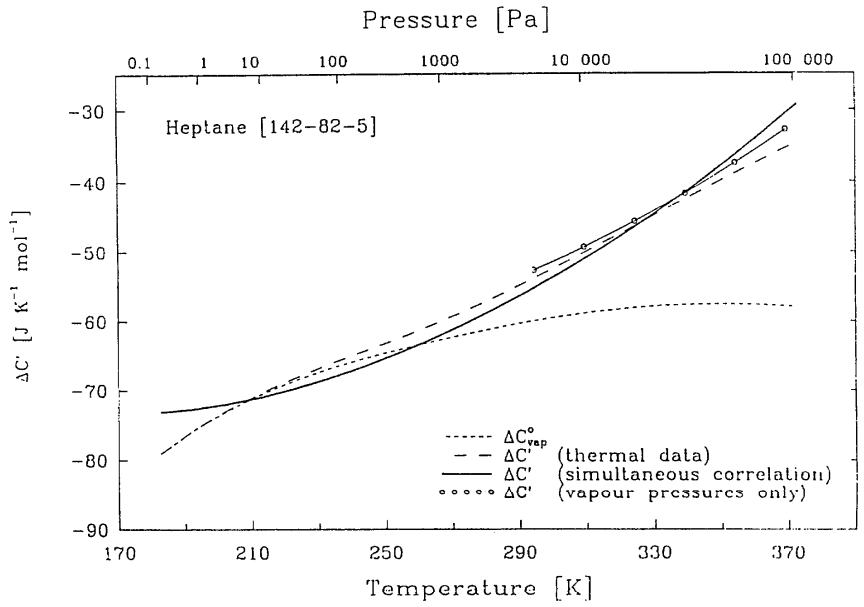

FIG. 1. Variation of $\Delta C'$ and ΔC°_{vap} with temperature

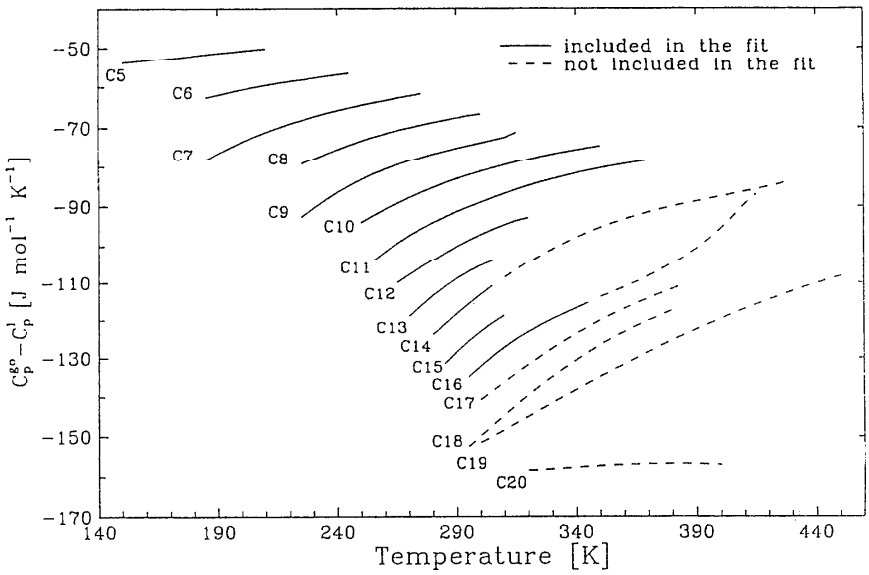

FIG. 2. Heat capacity difference ΔC°_{vap} of n-alkanes as a function of temperature.

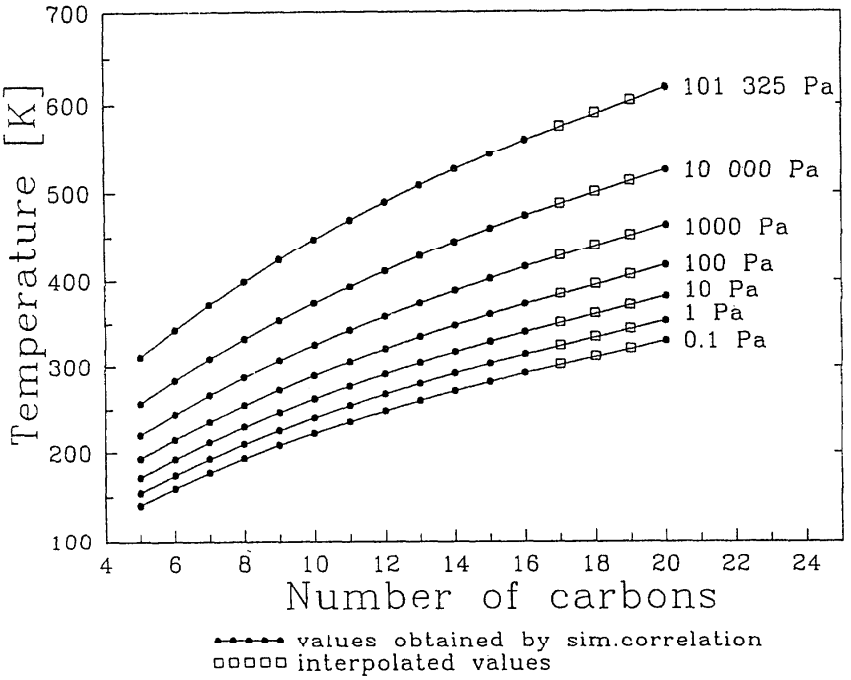

FIG. 3. Equilibrium temperatures plotted against the number of carbon atoms at different vapor pressures.

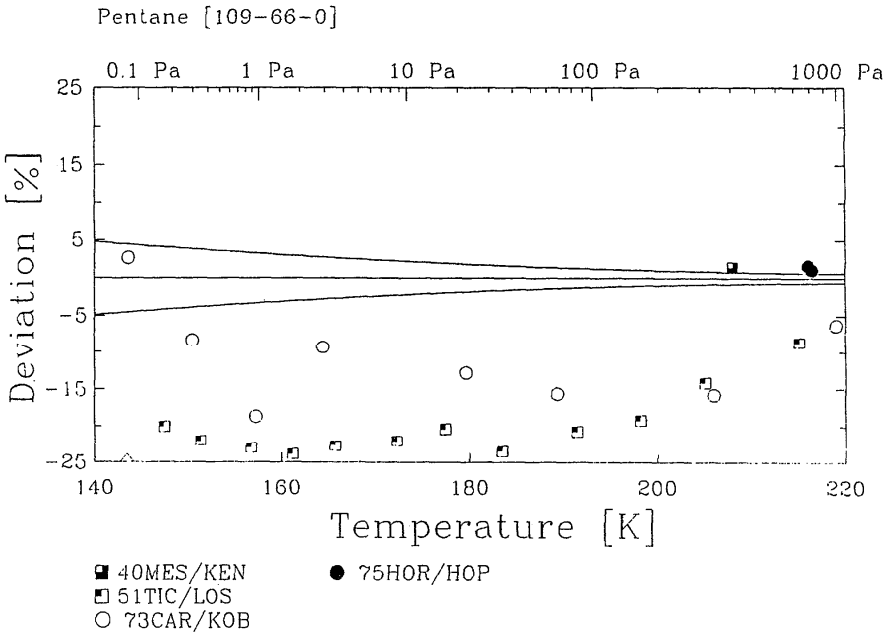

FIG. 4. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for pentane.

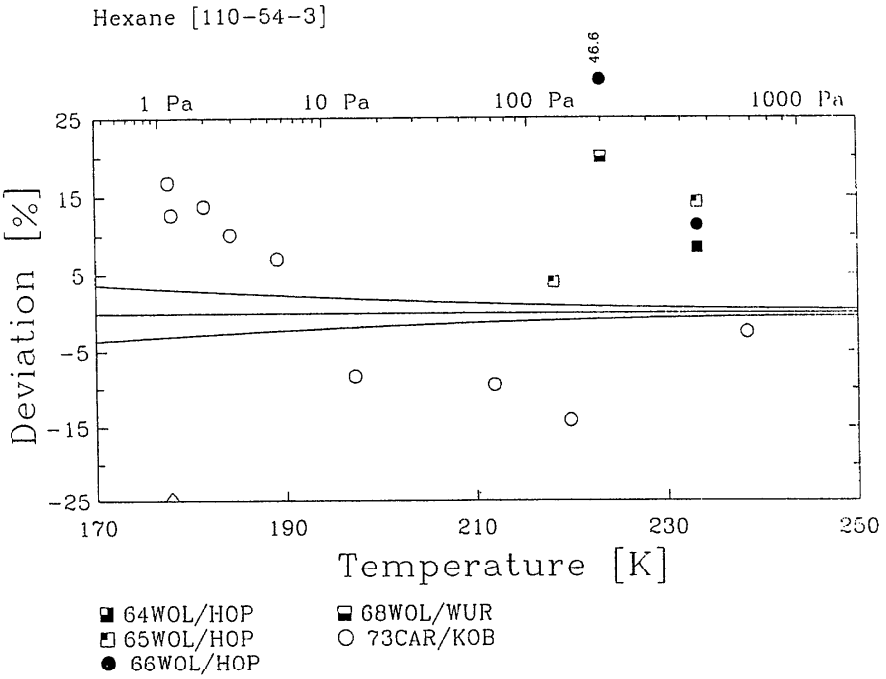

FIG. 5. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for hexane.

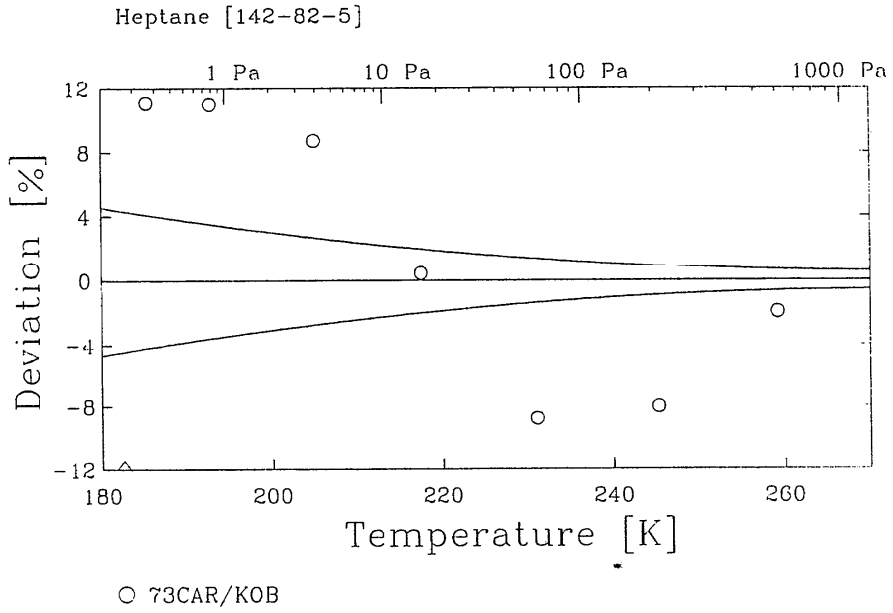

FIG. 6. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for heptane .

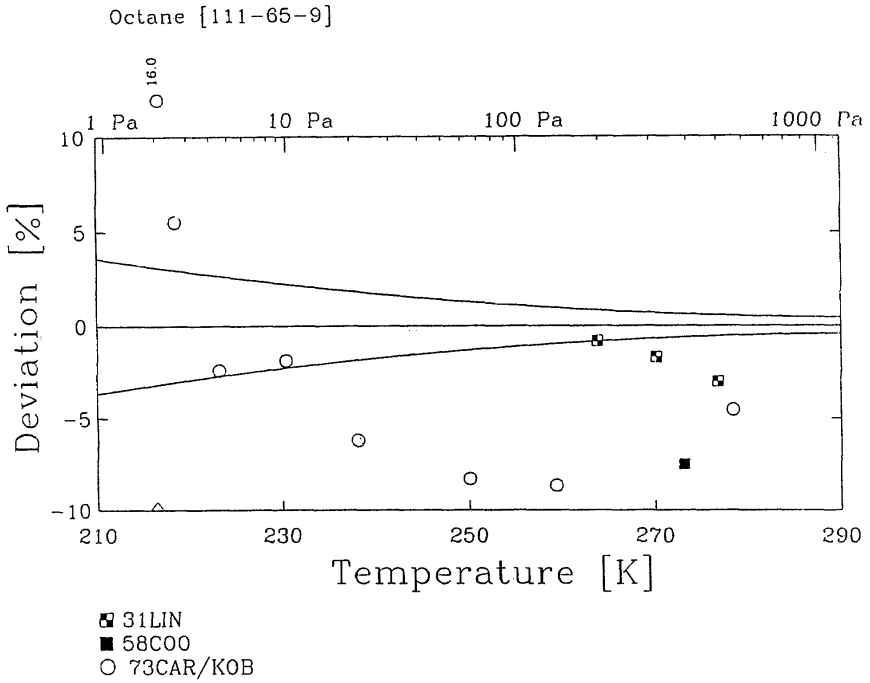

FIG. 7. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for octane.

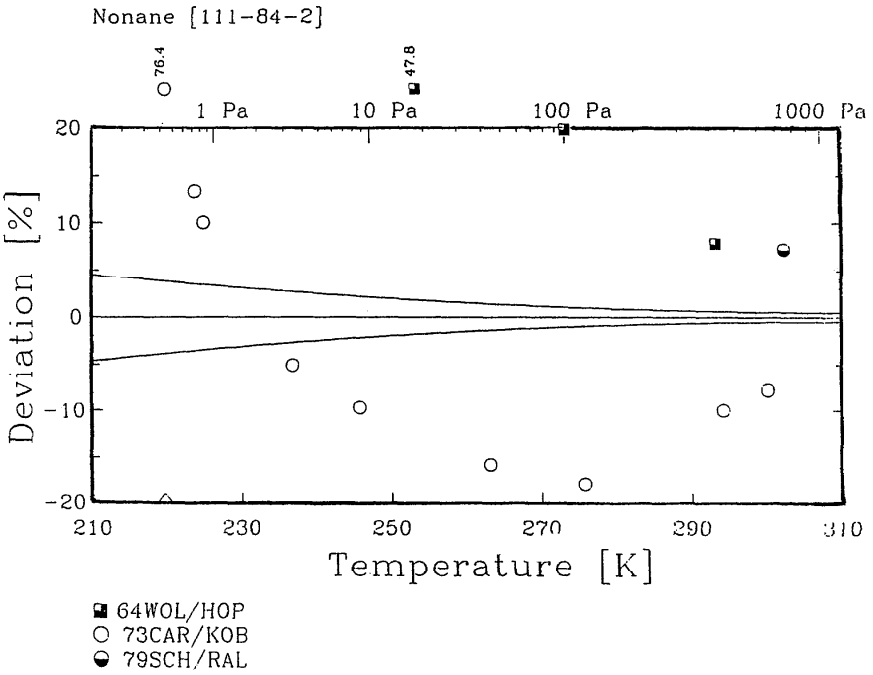

FIG. 8. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for nonane.

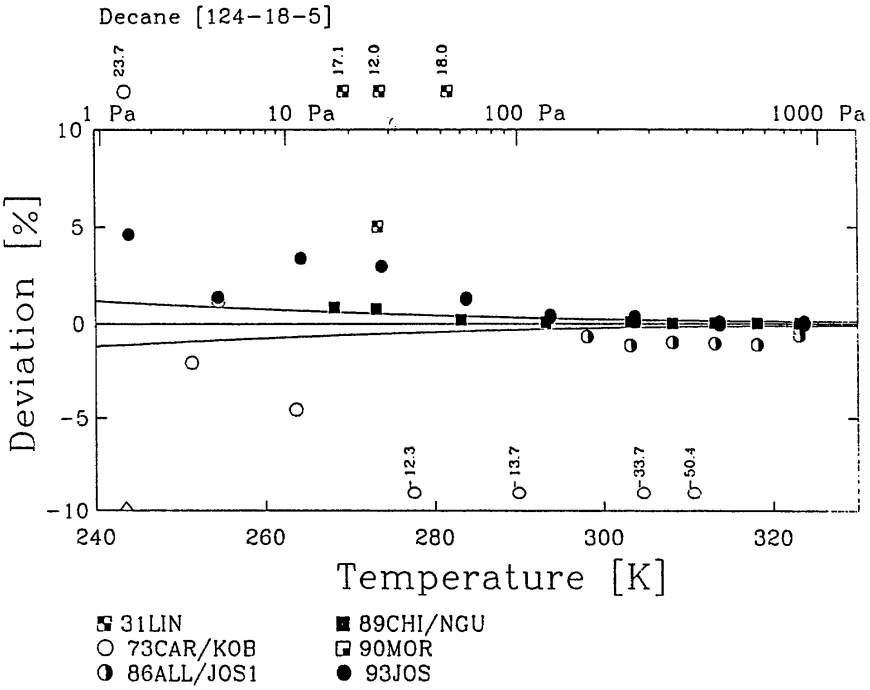

FIG. 9. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for decane.

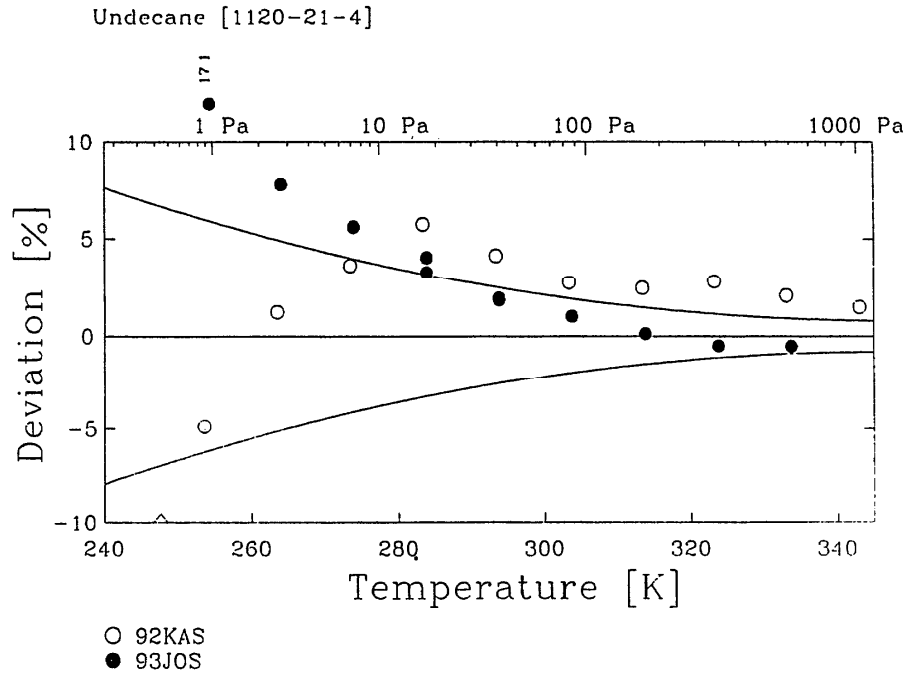

FIG. 10. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for undecane.

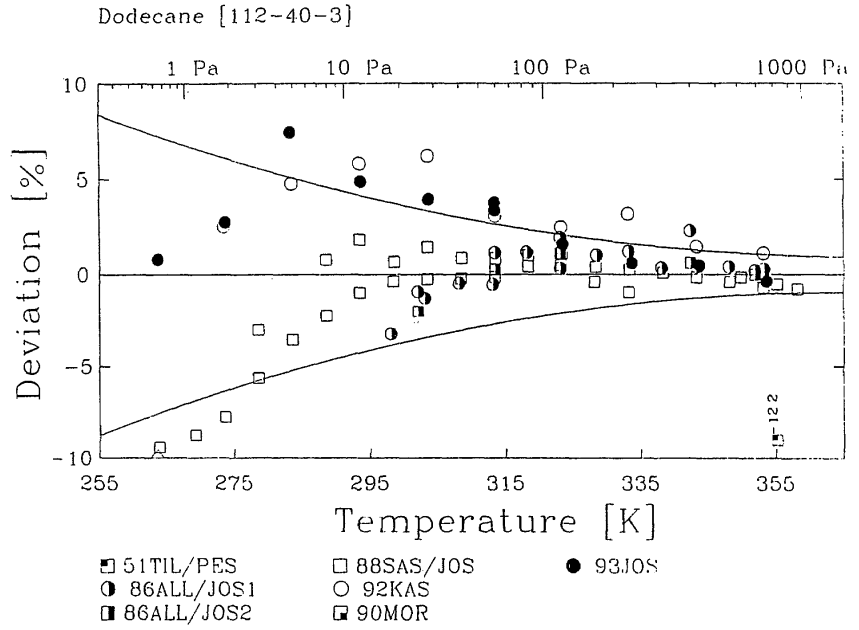

FIG. 11. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for dodecane.

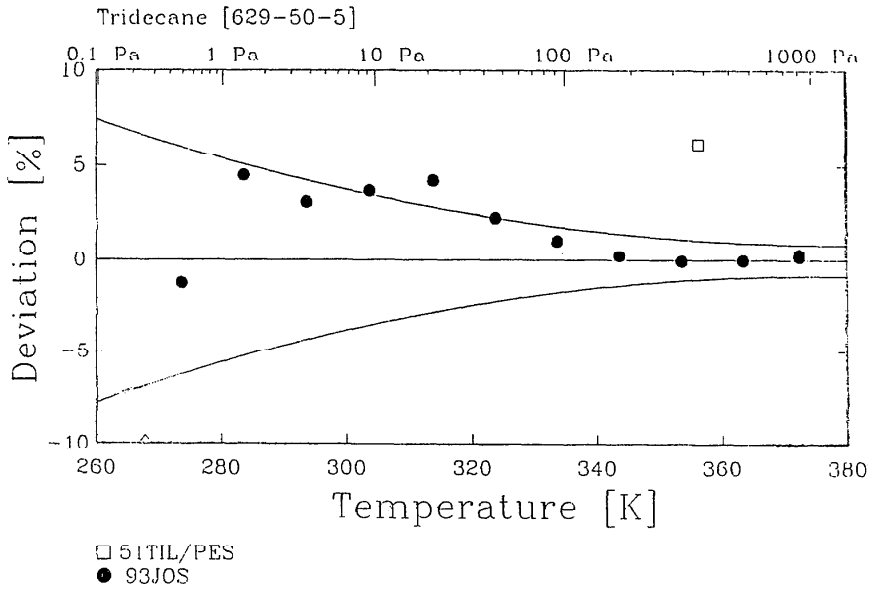

FIG. 12. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for tridecane.

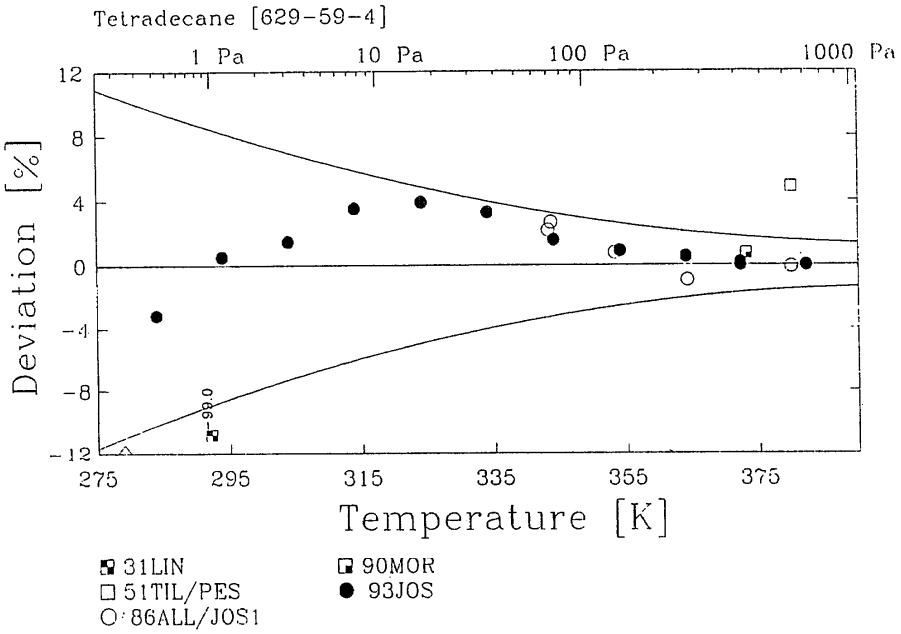

FIG. 13. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for tetradecane.

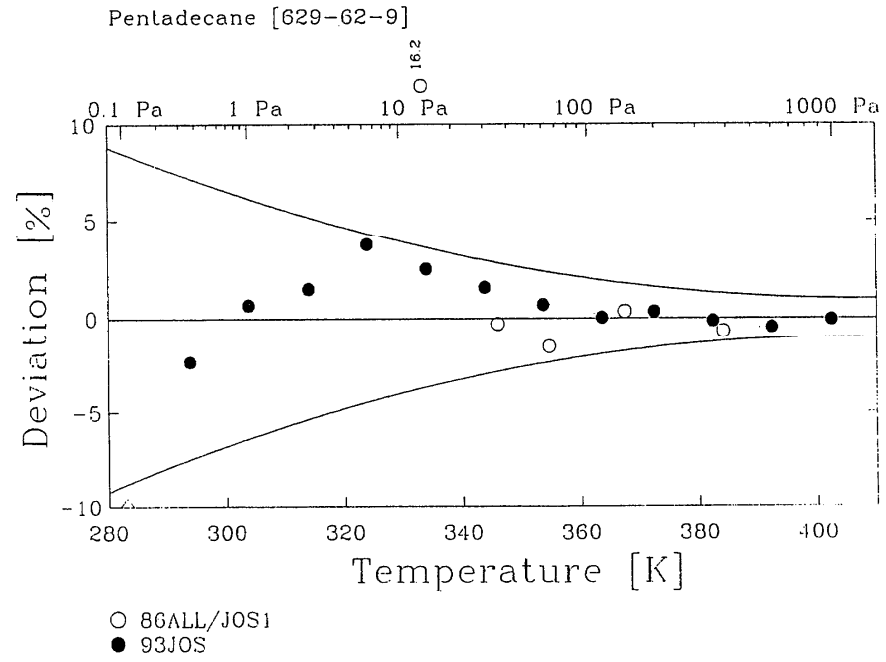

FIG. 14. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for pentadecane.

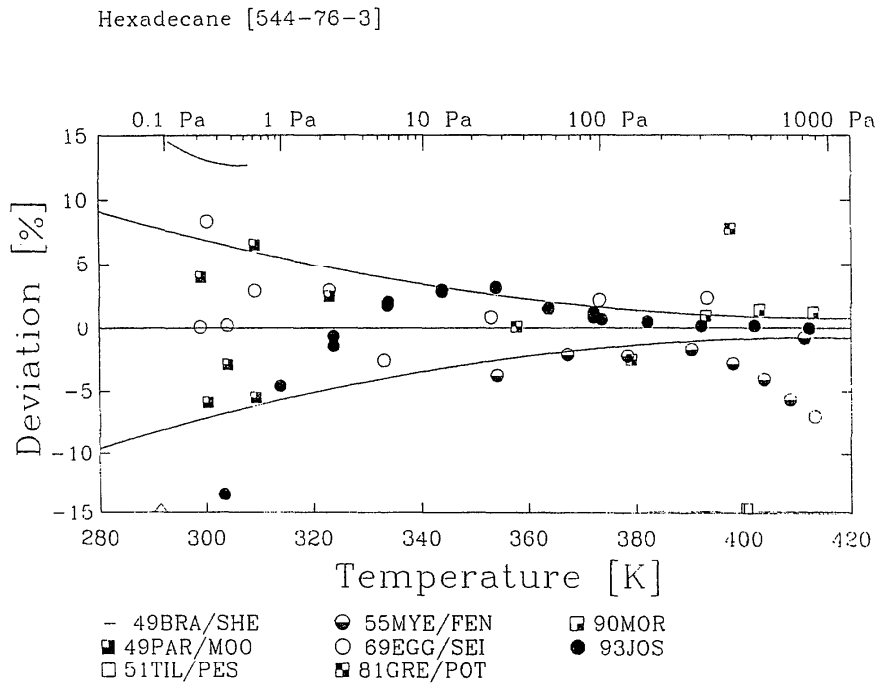

FIG. 15. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for hexadecane.

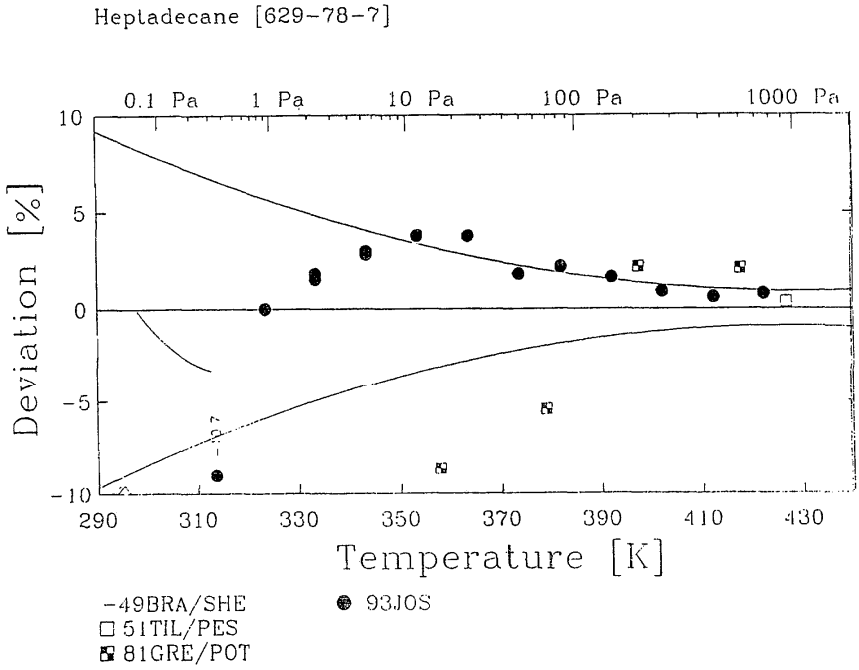

FIG. 16. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for heptadecane.

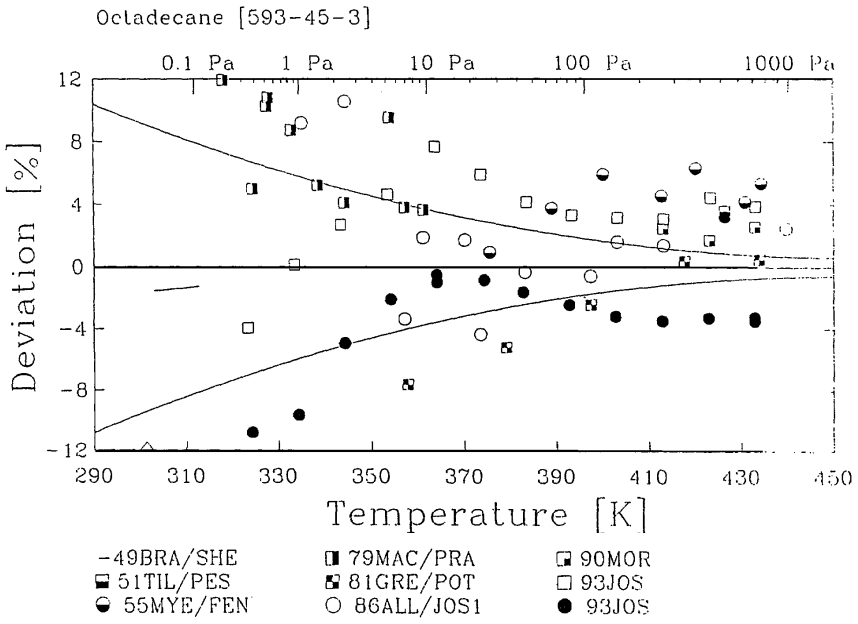

FIG. 17. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for octadecane.

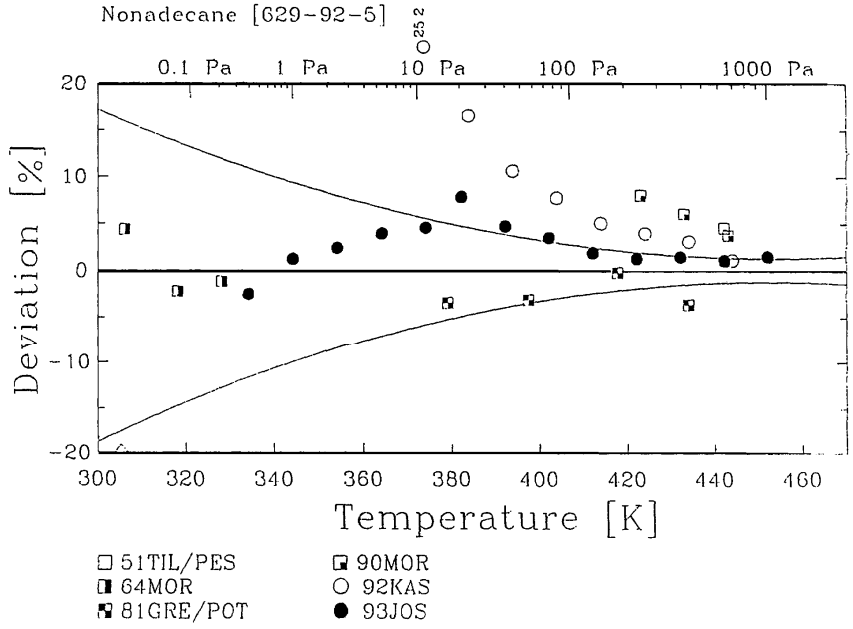

FIG. 18. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for nonadecane.

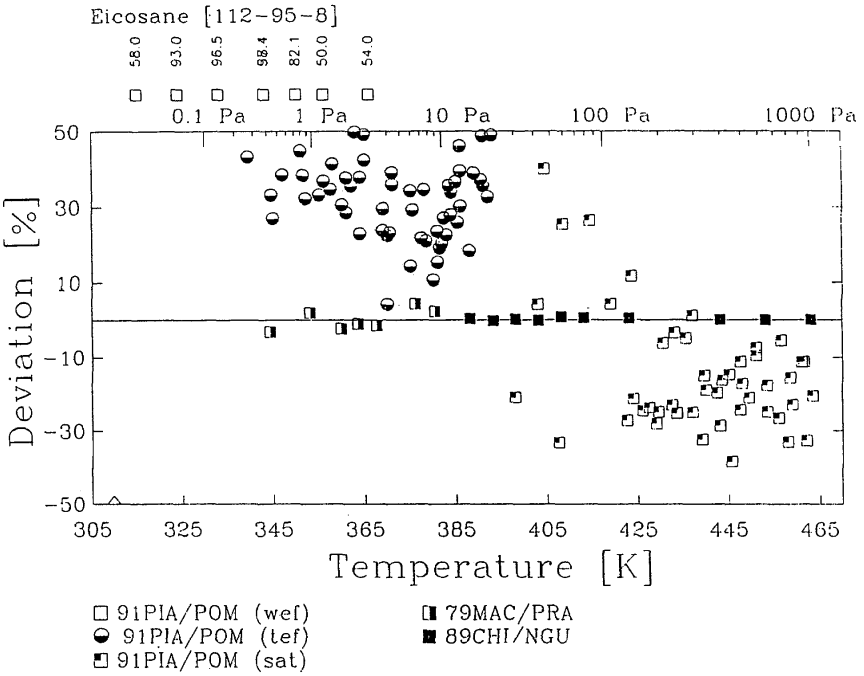

FIG. 19a. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for eicosane.

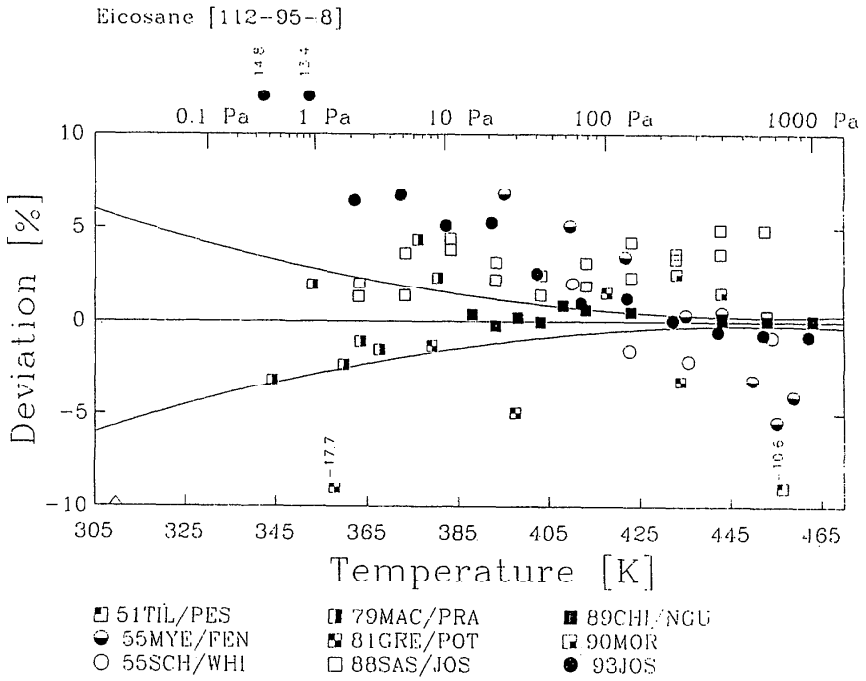

FIG. 19b. Deviations of experimental p_{sat} values from the recommended values below 1 kPa for eicosane.

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