Critical Properties and Vapor Pressure Equation for Alkanes C_nH_{2n+2}: Normal Alkanes With $n \leqslant 36$ and Isomers for $n=4$ Through $n=9$

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A correlation for estimating the vapor pressure of normal alkanes from methane through n-hexatriacontane and isomers of butane to nonane is reported. This work extends the correlation for normal alkanes (C_nH_{2n+2}), with $n \leqslant 20$, reported by Ambrose, to both normal alkanes with $n \leqslant 36$ and their isomers with $n \leqslant 9$. This vapor pressure equation was based on the Wagner equation and is similar to that used by Ambrose. Literature vapor pressure measurements have been reviewed. Tables are given that list the type of apparatus, measurement range and precision, and chemical purity. These criteria were initially used to select measurements for inclusion in the regression analyses to determine the coefficients of the correlation. Vapor pressures estimated from the correlation were compared with all vapor pressure (p^{1+g}) measurements reviewed in this work. At pressures greater than 1 kPa, the vapor pressure equation presented here has the following accuracies: $0.0001 \cdot p^{1+g}$ for methane, $0.001 \cdot p^{1+g}$ for ethane, propane, and n-butane, $0.002 \cdot p^{1+g}$ for n-pentane through n-octane, 2-methylpropane, and 2-methylbutane, $0.005 \cdot p^{1+g}$ for 2,2-dimethylpropane, n-nonane, n-decane, and the isomers of hexane through nonane, $0.01 \cdot p^{1+g}$ for n-undecane to n-hexadecane, $0.02 \cdot p^{1+g}$ for n-heptadecane to n-eicosane, $0.05 \cdot p^{1+g}$ for n-heneicosane to n-octacosane, and $0.10 \cdot p^{1+g}$ for n-nonacosane to n-hexatriacontane. Equations for the critical temperatures and pressures of the normal alkanes as functions of the carbon number are also reported. © *2000 American Institute of Physics.* [S0047-2689(90)00201-X]

Key words: alkane isomers, branched alkanes, critical pressure, critical temperature, hydrocarbons, normal alkanes, vapor pressure.

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1. Introduction

Numerous equations can be used to represent the vapor pressure p^{1+g} of a pure fluid (e.g., Ambrose, 1980, 1986, Ambrose and Tsonopoulos, 1995, Iglesias-Silva *et al.*, 1987, Ruzicka and Majer, 1996). Of particular significance is the empirical equation

$$\ln\left(\frac{p^{1+g}}{p_c}\right)=\frac{1}{T_r}\sum_i a_i\tau^{i/2}, \tag{1}$$

proposed by Wagner (1974) and Wagner *et al.* (1976) where

$$\tau=1-T_r \text{ and } T_r=\frac{T}{T_c}. \tag{2}$$

The subscript c identifies the critical condition and the a_i are adjustable parameters determined by regression analysis. The critical pressure and temperature are incorporated in the vapor pressure equation as reducing parameters. Section 2 provides an analysis of the critical temperatures and pressures of the normal alkanes used for these parameters. The coefficients and the particular functional form of Eq. (1) were determined with statistical methods.

The functional form presented in Eq. (1) can be written as

$$p^{1+g}=p_c\exp\left(\frac{1}{T_r}\sum_i a_i\tau^{i/2}\right)=p_c e^A, \tag{3}$$

where A is the right side of Eq. (1). At the critical point, τ is 0, and the vapor pressure is

$$p^{1+g}|_{T=T_c}=p_c e^{a_0}, \tag{4}$$

so that a_0 must be equal to zero. Likewise, the index i must be either 0 or positive so that p^{1+g} will not be infinite at the critical point. The slope of the vapor pressure equation is given by

$$\mathrm{d}p^{1+g}/\mathrm{d}T=p_c(\mathrm{d}A/\mathrm{d}T)e^A, \tag{5}$$

where

$$\mathrm{d}A/\mathrm{d}T=-\frac{1}{T_rT}\sum_i a_i\tau^{i/2}-\frac{1}{2T}\sum_i ia_i\tau^{(i-2)/2}. \tag{6}$$

At the critical temperature, the slope of the vapor pressure equation is

$$\mathrm{d}p^{1+g}/\mathrm{d}T|_{T=T_c}=-\frac{p_c}{T_c}(a_0+0.5a_1\tau^{-1/2}+a_2)e^{a_0}. \tag{7}$$

The value of a_1 must be 0 to prevent the slope of the vapor pressure curve from becoming infinite at the critical point. Since $a_0=0$ and the value of $\mathrm{d}p^{1+g}/\mathrm{d}T$ must be positive at the critical point, the value of a_2 must be negative. At the critical point, $\mathrm{d}\ln(p^{1+g})/\mathrm{d}\ln(T)=\alpha_c$, the parameter on which Riedel (1954) based his corresponding states scheme. For most substances, α_c (which is equivalent to $-a_2$) lies between 6 and 8.

The curvature of the vapor pressure equation must tend toward infinity as T goes to T_c, the critical point, in order to exhibit the theoretically predicted nonanalytical behavior (Wagner, 1973). The curvature is given by

$$\mathrm{d}^2p^{1+g}/\mathrm{d}T^2=p_c(\mathrm{d}^2A/\mathrm{d}T^2)e^A+p_c(\mathrm{d}A/\mathrm{d}T)^2e^A, \tag{8}$$

where

$$\mathrm{d}^2A/\mathrm{d}T^2=\frac{2}{T_rT^2}\sum_i a_i\tau^{i/2}+\frac{1}{T^2}\sum_i ia_i\tau^{(i-2)/2}+\frac{1}{TT_c}\sum_i\frac{i(i-2)}{4}a_i\tau^{(i-4)/2}. \tag{9}$$

At the critical point,

$$\mathrm{d}^2p^{1+g}/\mathrm{d}T^2|_{T=T_c}=\frac{p_c}{T_c^2}[2a_2+0.75a_3\tau^{-1/2}+2a_4+a_2^2]e^{a_0}. \tag{10}$$

Since a_2 must be negative, either a_4 must be positive and large or a_3 must be positive. In nearly all cases, a_4 is set to 0, and a_3 is between 1 and 2.5.

Ambrose and Walton (1989) have shown that Eq. (1) in the form

$$\ln\left(\frac{p^{1+g}}{p_c}\right)=\frac{1}{T_r}(a_2\tau+a_3\tau^{1.5}+a_5\tau^{2.5}+a_{10}\tau^5) \tag{11}$$

with $a_2<0$ and $a_3>0$ is adequate to accommodate experimental results over a wide temperature and pressure range for most fluids. More recently Ewing and Sanchez Ochoa (1998) have shown that Eq. (11) can be used to extrapolate precise vapor pressure measurements at modest pressures (in this case below 0.5 p_c) to the critical point, provided that the critical temperature is known.

For methane and n-butane and to some extent for ethane and propane, there are adequate measurements over a sufficiently wide temperature range to obtain the coefficients of Eq. (11) for each fluid that provide accurate representations of the measurements. However, for other alkanes, most of the vapor pressure measurements were obtained near the normal boiling point, and often there are either very few or no vapor pressure data up to the critical temperature. The critical region is often uncertain particularly for the higher homologs. Thus a generalized equation is desirable to interpolate between measurements and assist in assessing the reliability of different data sets. Elsewhere, Ambrose and Walton (1989) discuss, for a particular homologous series, both the need for and the requirements of a generalized vapor pressure equation of the type defined by Eq. (11). In addition, a generalized vapor pressure equation can provide vapor pressure estimates where measurements are not available.

Ambrose and Walton (1989) developed a generalized vapor pressure equation for the normal alkanes C_nH_{2n+2}, with the number of carbon atoms $n\leqslant 20$, given by

$$\ln\left(\frac{p^{1+g}}{p_c}\right)=\frac{1}{T_r}(\mathrm{Pr}^{(0)}+\omega\mathrm{Pr}^{(1)}+\omega^2\mathrm{Pr}^{(2)}), \tag{12}$$

where $\mathrm{Pr}^{(0)}$, $\mathrm{Pr}^{(1)}$, and $\mathrm{Pr}^{(2)}$ are functions, based on Eq. (11), of τ given by

$$\mathrm{Pr}^{(0)}=N_1\tau+N_2\tau^{1.5}+N_3\tau^{2.5}+N_4\tau^5, \quad (13)$$

$$\mathrm{Pr}^{(1)}=N_5\tau+N_6\tau^{1.5}+N_7\tau^{2.5}+N_8\tau^5, \quad (14)$$

and

$$\mathrm{Pr}^{(2)}=N_9\tau+N_{10}\tau^{1.5}+N_{11}\tau^{2.5}+N_{12}\tau^5. \quad (15)$$

The parameter ω is similar, but not identical, to the acentric factor defined in Sec. 4. The values of ω used in this work are discussed in Sec. 4. Equation (12) was adopted here to represent the vapor pressures of normal alkanes and their isomers. The coefficients of Eqs. (13), (14), and (15) obtained in this work are given in Sec. 4.

Morgan and Kobayashi (1992) used several approaches to represent the vapor pressures of hydrocarbons with $n\leq 50$, including a form similar to Eq. (12) and a real fluid corresponding states model modified from that reported by both Pitzer *et al.* (1955) and Lee and Kesler (1975). Edalat *et al.* (1993) described a generalized vapor pressure equation based on Eq. (11) with correlations for each coefficient as functions of Pitzer's acentric factor. This approach was applied to n-alkanes, aromatics, halogens, alcohols and other nonhydrocarbons. For normal alkanes, Edalat *et al.* cite that their vapor pressure equation has an average uncertainty of $0.055\cdot p^{1+g}$. There are other generalized vapor pressure correlations in the literature for alkanes (e.g., Ambrose and Patel, 1984, Campanella, 1997, Gomez-Nieto and Thodos, 1978, Magoulas and Tassios, 1990), some of which use empirical expressions with few adjustable coefficients. These methods will not be considered further here. Values of the vapor pressure obtained from both the correlation of Ambrose and Walton (1989) for $n\leq 20$ and the work of Morgan and Kobayashi for $n>20$ [from the model identical to Eq. (12)] are shown in Sec. 5, along with the experimental data, as deviations from the equation developed in this work.

2. Critical Properties

Many group contribution schemes (e.g., Kontogeorgis and Tassios, 1997, Nikitin *et al.*, 1996, Reid *et al.*, 1987, Somayajulu, 1989) and correlations are available in the open literature to estimate critical properties of fluids. The correlations of Tsonopoulos (1987) and Teja *et al.* (1990) are reviewed briefly since they form the basis for the correlations of critical temperature and pressure determined in this work. The expressions reported for the critical temperature and pressure by Tsonopoulos (1987) are

$$T_c/\mathrm{K}=959.98-\exp(6.815\,36-0.211\,145n^{2/3}) \quad (16)$$

and

$$p_c/\mathrm{MPa}=\exp(2.017\,18-0.274\,281n^{2/3}). \quad (17)$$

These equations are valid for n-alkanes with $n\geq 3$. At high n, the critical pressure given by Eq. (17) approaches 0. This was later revised in the work of Tsonopoulos and Tan (1993), which used a modified version of the Flory theory and treated the critical properties on an internally consistent basis. Although more theoretical in nature, we have not included comparisons here with our equations since their work was not used in the development of the equations reported here.

Teja *et al.* (1990) modified Eqs. (16) and (17) by adjusting the exponent in the regression and including a term to ensure the critical pressure equation had a nonzero limiting value at high carbon numbers. The equations reported by Teja *et al.* (1990) for the critical temperature and pressure are

$$T_c/\mathrm{K}=1143.8-\exp(7.159\,08-0.303\,158n^{0.469\,609}) \quad (18)$$

and

$$p_c/\mathrm{MPa}=0.842\,03+\exp(1.750\,59-0.196\,383n^{0.890\,006}). \quad (19)$$

These equations are also valid for $n\geq 3$. Tsonopoulos (1987) indicated that the limiting values of T_c and p_c at very high carbon numbers may not be physically significant.

2.1. Critical Temperature for the Normal Alkanes

Recently, Ambrose and Tsonopoulos (1995) (see also Ambrose and Young, 1995) have reviewed and listed all available measurements for the critical temperatures and critical pressures for the normal alkanes from methane to tetracosane and reported recommended values for each substance up to octadecane. The critical temperatures recommended by Ambrose and Tsonopoulos were fitted here as a function of carbon number, $n<18$, to the equation

$$T_c/\mathrm{K}=a_1-\exp(a_2+a_3n^{a_4}+\gamma a_5/n^5), \quad (20)$$

where $\gamma=1$ for even carbon numbers and $\gamma=0$ for odd carbon numbers. Equation (20) was based on the work of Teja *et al.* (1990) with the addition of the term $\gamma a_5/n^5$. This term accounts for the differences in critical properties of alkanes with even and odd carbon numbers with n less than 8. The contribution of $\gamma a_5/n^5$ is significant for ethane (for which it amounts up to $0.025\cdot T_c$) and n-butane, less significant for n-hexane, and has an insignificant contribution to the values of T_c determined for n-octane and higher alkanes with even carbon numbers. This even–odd effect has apparently been ignored throughout the literature, i.e., most prior correlations start with n between 3 and 5, and the properties of methane, ethane, and often propane and n-butane are not included in the correlations. However, Malanoski and Monson (1999) discuss its effect with respect to the ratio of the triple point temperature to the critical point temperature. The coefficients of Eq. (20), given in Table 1, were determined using a nonlinear regression of selected critical temperatures.

Differences between the values of T_c obtained from Eq. (20) and the values recommended by Ambrose and Tsonopoulos are shown in Fig. 1, as well as the differences between the values of T_c obtained from Eq. (20) and the critical temperatures determined from both the correlations of Teja *et al.* (1990) and Tsonopoulos (1987). For $n>18$, the only source of critical parameters are those reported by Nikitin *et al.* (1994), (1997). The top of Fig. 1 shows deviations for n

TABLE 1. Coefficients a_i of Eq. (20) for T_c, b_i of Eq. (21) for p_c, and c_i of Eq. (24) for ω

i	a_i	b_i	c_i
1	1200.	0.734 993 18	3.0
2	7.235 346 1	2.115 168 4	1.155 678 7
3	−0.318 197 03	−0.362 293 42	−0.053 002 297
4	0.436 006 96	0.691 231 21	0.616 912 28
5	−0.269 056 63	−0.220 560 59	
6		−2.889 041 6	

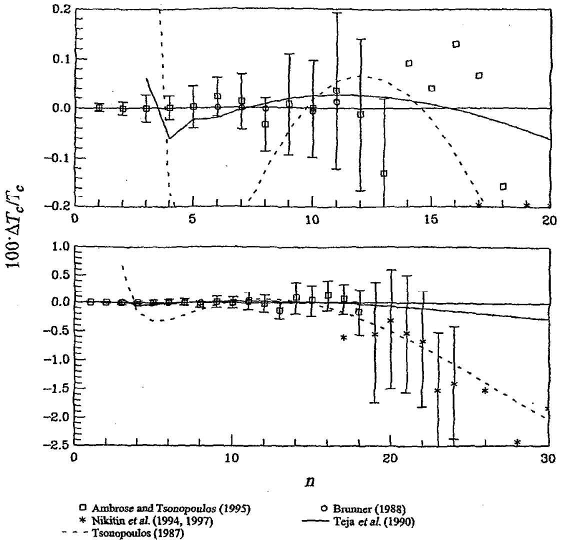

FIG. 1. Percent deviations of experimental critical temperatures from values obtained from Eq. (20) as a function of the number of carbon atoms n for C_nH_{2n+2} with $n \leqslant 20$ and $n \leqslant 30$.

<20 on a scale of $\pm 0.002 \cdot T_c$, while the lower figure shows values for $n<30$ on a scale from $-0.025 \cdot T_c$ to $+0.01 \cdot T_c$. The uncertainties in the critical properties shown in Fig. 1 are those reported by Ambrose and Tsonopoulos.

For methane through n-pentane, Eq. (20) represents the values of T_c reported by Ambrose and Tsonopoulos and coworkers within $0.000\,02 \cdot T_c$, while for n-hexane, n-heptane, and n-octane, the differences between the recommendations and Eq. (20) are less than $0.0004 \cdot T_c$. However, Eq. (20), as shown in Fig. 1, represents the critical temperatures for n-hexane, n-heptane, and n-octane reported by Brunner (1988) within $0.000\,02 \cdot T_c$. Although the values recommended by Ambrose and Tsonopoulos for n-hexane, n-heptane, and n-octane were used initially to adjust the coefficients of Eq. (20), the values of T_c reported by Brunner, including that for n-undecane, were used in the final determination of the parameters in Eq. (20), as there was a significant reduction in the standard deviation of the fit and an improved representation of the critical temperatures for all alkanes. The value of the critical temperature for n-nonane determined by Brunner is not shown in Fig. 1, nor included in the analysis discussed here, since its deviation from Eq. (20) is more than a factor of 10 greater than that for the other alkanes. The values reported by Brunner for n-hexane, n-heptane, and n-octane are used throughout the remainder of this work. For n-nonane and higher alkanes, the critical temperatures determined from Eq. (20) were used in this work and are listed in Table 2. These numbers were determined from an analysis that was very different from that used by Ambrose and Tsonopoulos. Their work was based solely on experimental evidence, with no smoothing as done here. Although the experimental values have associated uncertainties, there is no clear evidence that the molecular structure of the normal alkanes is such that a smooth function of critical temperature or pressure will result as a function of carbon number, and the differences seen in Fig. 1 may not be due to experimental error. Thus, judgment must be used in the selection of critical properties for different applications.

Also shown in Fig. 1 are the values of the critical temperatures for the alkanes $C_{17}H_{36}$ through $C_{30}H_{62}$ reported by Nikitin *et al.* (1994), (1997). These are the only available measurements for the critical parameters of $C_{19}H_{40}$ and higher of which we are aware. The critical temperature for $C_{17}H_{36}$ reported by Nikitin *et al.* lies $0.005 \cdot T_c$ below the value recommended by Ambrose and Tsonopoulos; this is twice the estimated uncertainty given by Ambrose and Tsonopoulos. The thermal stability of these higher alkanes decreases with increasing n and it is plausible that the other values reported by Nikitin have uncertainties greater than $0.005 \cdot T_c$ at higher values of n. Consequently, the critical temperature values reported by Nikitin *et al.* were not used in the fit. Additional measurements of the critical properties of n-alkanes for $n>20$ are needed to validate these conclusions.

The correlation for T_c reported by Teja *et al.* (1990) and given by Eq. (18) differs from Eq. (20) by no more than $0.0003 \cdot T_c$ for $4<n \leqslant 18$ and by less than $0.003 \cdot T_c$ for $18<n \leqslant 30$, much less than the experimental uncertainty for these carbon numbers. Teja *et al.* did not make any correction for the lower alkanes using an even–odd type term. The equation of Tsonopoulos (1987) follows the trends set by the data of Nikitin *et al.* at higher carbon numbers. For the lower alkanes, the equation of Tsonopoulos shows deviations greater than the assigned uncertainty from the recommendations of Ambrose and Tsonopoulos, with differences exceeding $-0.001 \cdot T_c$ for $n<9$. The upper limit of Eq. (20) is 1200 K. The maximum temperatures for the literature correlations of T_c are 1143.8 K for Teja *et al.* and 959.98 K for Tsonopoulos.

2.2. Critical Pressure for the Normal Alkanes

An empirical approach, similar to that described above for critical temperatures, was adopted to correlate the values of p_c recommended by Ambrose and Tsonopoulos (1995) for the n-alkanes. The best representation was found to be

$$p_c/\mathrm{MPa} = b_1 + \exp[b_2 + b_3 n^{b_4} + b_5/n + \zeta b_6/(n+1)^4], \quad (21)$$

TABLE 2. Values of T_c, p_c, and ω for the normal alkanes used in Eq. (12)

n	Substance	Reference	T_c/K[a]	p_c/MPa[b]	ω	T_b/K[c]
1	Methane	Setzmann and Wagner (1991)	190.564	4.5992	0.011 41	111.668
2	Ethane	Douslin and Harrison (1973)	305.322	4.8718	0.105 74	184.561
3	Propane	Thomas and Harrison (1982)	369.825	4.2462	0.158 13	230.980
4	*n*-Butane	Ambrose and Tsonopoulos (1995)	425.12	3.7861	0.203 54	272.644
5	*n*-Pentane	Ambrose and Tsonopoulos (1995)	469.70	3.3665	0.250 71	309.195
6	*n*-Hexane	Brunner (1988)	507.49	3.0181	0.294 11	341.852
7	*n*-Heptane	Brunner (1988)	540.13	2.727	0.336 02	371.534
8	*n*-Octane	Brunner (1988)	568.88	2.486	0.376 50	398.783
9	*n*-Nonane		594.55	2.281	0.414 03	423.882
10	*n*-Decane		617.7	2.103	0.449 49	447.225
11	*n*-Undecane		638.8	1.950	0.483 15	469.029
12	*n*-Dodecane		658.1	1.817	0.515 24	489.439
13	*n*-Tridecane		675.9	1.700	0.545 93	508.658
14	*n*-Tetradecane		692.4	1.599	0.575 36	526.740
15	*n*-Pentadecane		707.7	1.510	0.603 66	543.782
16	*n*-Hexadecane		722.1	1.432	0.630 92	559.975
17	*n*-Heptadecane		735.5	1.363	0.657 24	575.244
18	*n*-Octadecane		748.2	1.301	0.682 69	589.844
19	*n*-Nonadecane		760.1	1.247	0.707 34	603.618
20	*n*-Eicosane		771.4	1.198	0.731 24	616.799
21	*n*-Heneicosane		782.1	1.155	0.754 45	629.319
22	*n*-Docosane		792.2	1.116	0.777 00	641.231
23	*n*-Tricosane		801.9	1.082	0.798 95	652.633
24	*n*-Tetracosane		811.1	1.051	0.820 32	663.513
25	*n*-Pentacosane		819.9	1.023	0.841 15	673.940
26	*n*-Hexacosane		828.3	0.997	0.861 46	683.949
27	*n*-Heptacosane		836.3	0.975	0.881 30	693.429
28	*n*-Octacosane		844.0	0.954	0.900 67	702.607
29	*n*-Nonacosane		851.	0.936	0.919 61	711.034
30	*n*-Triacontane		858.	0.919	0.938 13	719.396
31	*n*-Hentriacontane		865.	0.903	0.956 25	727.693
32	*n*-Dotriacontane		872.	0.889	0.974 00	735.866
33	*n*-Tritriacontane		878.	0.877	0.991 38	743.062
34	*n*-Tetratriacontane		884.	0.865	1.008 42	750.243
35	*n*-Pentatriacontane		890.	0.855	1.025 12	757.287
36	*n*-Hexatriacontane		896.	0.845	1.041 50	764.314
37	*n*-Heptatriacontane		901.	0.837	1.057 58	770.347
38	*n*-Octatriacontane		907.	0.829	1.073 36	777.217
39	*n*-Nonatriacontane		912.	0.821	1.088 85	783.214
40	*n*-Tetracontane		917.	0.815	1.104 07	789.064
41	*n*-Hentetracontane		922.	0.809	1.119 03	794.897
42	*n*-Dotetracontane		926.	0.803	1.133 73	799.849
43	*n*-Tritetracontane		931.	0.798	1.148 18	805.581

[a] Values of the critical temperatures for *n*-nonane and above were determined from Eq. (20).

[b] Values of the critical pressures for propane through *n*-octane were determined in the regression analysis described in Sec. 4.1. Values for *n*-nonane and above were calculated from Eq. (21).

[c] Calculated from Eq. (12) at 0.101 325 MPa.

where $\zeta=0$ for even carbon numbers and $\zeta=1$ for odd carbon numbers. The coefficients b_1 through b_6, which were determined by regression analysis to selected critical pressures, are listed in Table 1. Equation (21) is based on the work of Teja *et al.* (1990) with the addition of the terms b_5/n and $\zeta b_6/(n+1)^4$. The value of $\zeta b_6/(n+1)^4$ is significant for methane and propane, and less significant for *n*-pentane and higher *n*-alkanes with odd carbon numbers.

The values of p_c recommended by Ambrose and Tsonopoulos and those calculated from the critical pressure correlations of Teja *et al.* (1990) [Eq. (19)] and Tsonopoulos (1987) [Eq. (17)] are shown in Fig. 2 as deviations from Eq. (21). The top of Fig. 2 shows deviations for $n<20$ on a scale of $\pm 0.03 \cdot p_c$, while the lower curve shows values for $n<30$ on a compressed ordinate scale of $-0.25 \cdot p_c$ to $+0.05 \cdot p_c$. The uncertainties in critical pressures shown in Fig. 2 are those reported by Ambrose and Tsonopoulos. With the exception of $C_{24}H_{50}$, Eq. (21) represents the recommended values within their reported uncertainties.

For methane, ethane, propane, *n*-hexane, and *n*-octane, Eq. (21) represents the values reported by Ambrose and Tsonopoulos within $0.0003 \cdot p_c$. For *n*-butane, *n*-pentane, and *n*-heptane, the differences are as high as $0.003 \cdot p_c$. However, the critical pressures of *n*-butane and *n*-pentane reported by Kratzke *et al.* (1982), (1985) lie within $0.0006 \cdot p_c$, while those for *n*-heptane determined by Brunner lie

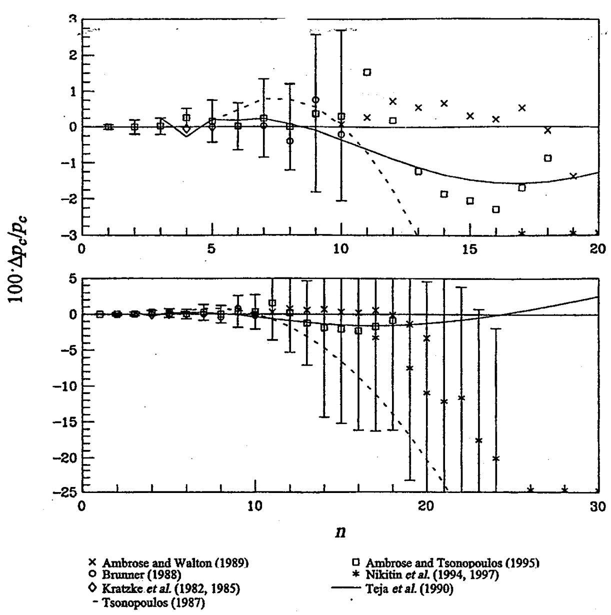

FIG. 2. Percent deviations of experimental critical pressures from values obtained from Eq. (21) as a function of the number of carbon atoms n for C_nH_{2n+2} with $n \leqslant 20$ and $n \leqslant 30$.

fractionally above Eq. (21) by $0.0003 \cdot p_c$, similar to that for n-hexane.

For $C_{11}H_{24}$ the value of p_c recommended by Ambrose and Tsonopoulos differs by about $0.015 \cdot p_c$ from Eq. (21) and consequently was not used in the fit. For $C_{13}H_{26}$ and higher, the critical pressure values recommended by Ambrose and Tsonopoulos lie below Eq. (21) by more than $0.01 \cdot p_c$, but still within the uncertainty assigned by them. However, Ambrose and Walton (1989) developed a generalized vapor pressure correlation with critical pressures about $0.005 \cdot p_c$ greater than those calculated using Eq. (21). The values of p_c reported here were influenced by the global fitting of the vapor pressure correlation presented in Sec. 4. Values of p_c determined from Eq. (21) for n-nonane and higher were used in this work and are listed in Table 2.

Also shown in Fig. 2 are the values of the critical pressures for the alkanes $C_{17}H_{36}$ through $C_{30}H_{62}$ reported by Nikitin *et al.* (1994), (1997). These are the only measurements, of which we are aware, for the critical parameters of $C_{19}H_{40}$ and higher. The value of p_c for $C_{17}H_{36}$ reported by Nikitin *et al.* lies $0.015 \cdot p_c$ below the recommended value of Ambrose and Tsonopoulos and $0.032 \cdot p_c$ below Eq. (21). It is plausible, as it was with T_c, that the values of Nikitin are in error by more than $0.05 \cdot p_c$ for $n \geqslant 18$. Consequently, the values of p_c reported by Nikitin *et al.* were not used in the fit.

The values of p_c obtained from Eq. (21) differ from the correlation of Teja *et al.* [Eq. (19)] by less than $0.003 \cdot p_c$ for $3 \leqslant n \leqslant 9$ and by less than $0.016 \cdot p_c$ for $9 < n \leqslant 28$. No correction for the even–odd carbon numbers was used for the lower alkanes by Teja *et al.* The lower limit of Eq. (21) is 0.735 MPa. The literature correlations of p_c have minimum pressures of 0.842 03 MPa for Teja *et al.* (1990) and 0 for Tsonopoulos (1987).

Equations (20) and (21) represent the critical temperatu and pressure within their experimental uncertainty for alkanes below n-eicosane. We have assumed, based on both the consistency of the critical parameters for alkanes below n-eicosane with experimental data and the probable ability of the simple functions, Eqs. (20) and (21), to extrapolate to higher carbon numbers, that acceptable estimates of the critical temperature and pressure may be obtained for the higher alkanes from the correlations presented here. New measurements of the critical temperature and pressure are needed to verify this assumption and the representation of these properties reported here and previous correlations for $n \geqslant 20$.

3. Vapor Pressure Measurements from the Literature

Sources of vapor pressure measurements reporting more than one vapor pressure measurement for normal alkanes with $n \leqslant 43$ and isomers for $n = 4$ through 9 are listed in Table 3 together with the experimental technique used for the measurements, and the precision and accuracy cited for that technique by the authors. Descriptions for most of the experimental techniques have been reported by either Ambrose (1973), (1975) or Morgan and Kobayashi (1992), (1994). All literature data have been converted to ITS-90, the temperature scale used throughout this work (Preston-Thomas, 1990). In some cases where the authors did not cite an accuracy, it was estimated by comparisons with other data sets obtained with similar methods. In Table 4, the purity of the sample used for the measurements is provided along with the number of measurements, the minimum and maximum measured temperature and pressure, and the estimated uncertainty in measurements at the minimum and maximum temperature. Sources reporting only one data point per substance are not listed. Table 4 also lists the measurements used in the regression analyses described here. The total uncertainty Δp^{1+g} in the vapor pressure at both the minimum and maximum measured temperatures for each set of measurements was determined from

$$\Delta p^{1+g}=\left[\left(\frac{\Delta p_{\mathrm{expt}}}{p}\right)^2+\left(\frac{\Delta T_{\mathrm{expt}}}{p}\right)^2\left(\frac{\mathrm{d}p^{1+g}}{\mathrm{d}T}\right)^2\right]^{1/2}\cdot p, \tag{22}$$

where Δp_{expt} and ΔT_{expt} are the experimental uncertainties in pressure and temperature from Table 3, and $\mathrm{d}p^{1+g}/\mathrm{d}T$ was obtained from the correlation presented here. The uncertainties at the minimum and maximum temperatures generally correspond to the minimum and maximum uncertainties in p^{1+g}.

4. Vapor Pressure

4.1. *n*-Alkanes

The functional form developed by Ambrose, given in Eq. (12), and the values of the critical temperature (on ITS-90),

TABLE 3. Experimental methods used to determine vapor pressure, the precision and accuracy in temperature ΔT, the precision and accuracy in pressure Δp, and fluids studied

Author	Method[a]	ΔT/K[b]	Δp/kPa[b]	Fluids[c]
Abara *et al.* (1988)	1	0.01 {0.1}	13 {20}	6–8
Akimoto *et al.* (1984)	1	0.01	0.01	6
Allemand *et al.* (1986)	8	0.02	$0.01p$	10,12,14,15,18
Armstrong *et al.* (1955)	1	0.01	0.013 {$0.001-0.002p$}	1
Aston and Messerly (1936)	1	0.001	0.0013	5
Aston and Messerly (1940)	1	0.002	0.0013	4
Aston and Schumann (1942)	1	0.001	0.0008	5
Aston *et al.* (1940)	1	0.001	0.0013	4
Barber (1968)	1	0.05 {0.1}	2.1 {3.4}	3
Barclay *et al.* (1982)	1	0.01	$0.00013p+0.24$	2
Beale and Docksey (1935)	3	0.1	0.027	12
Beattie and Edwards (1948)	1		$0.0008p$	8
Beattie and Kay (1937)	1	0.01		7
Beattie *et al.* (1935a)	1	0.002	$0.0005p$	2
Beattie *et al.* (1935b)	1	0.005	$0.0003p$	3
Beattie *et al.* (1939)	1	0.001	0.051	4
Beattie *et al.* (1949)	1	1	0.1	4
Beattie *et al.* (1951a)	1			5
Beattie *et al.* (1951b)	1	0.05	0.0067	5
Beaudoin and Kohn (1967)	1	0.02	7.1	10
Bell *et al.* (1968)	1	0.02		6–8
Besserer and Robinson (1973a)	1	0.056	21	5
Besserer and Robinson (1973b)	1	0.056	1.4	4
Besserer and Robinson (1975a)	1	0.056	21	4
Besserer and Robinson (1975b)	1	0.056	21	5
Bich *et al.* (1992)	1	$0.000\,05T$	0.01	6
Bissell and Williamson (1975)	1	0.002	0.025	6,7
Bloomer and Parent (1953)	1	0.056	0.34	1
Bottomley and Reeves (1958)	1	0.01	0.0067	6
Brame and Hunter (1927)	3	0.1		5–8
Brooks *et al.* (1939)	3			8
Brooks *et al.* (1940)	3	0.003		6–8
Brown (1952)	6	0.01	0.0013	6,7
Brown *et al.* (1988)	1	0.02	$p<690$: 0.69, $690<p<3400$: 0.4, $p>3400$:17	2
Brown *et al.* (1989)	6	0.02	0.7	4
Bruun and Hicks-Bruun (1930)	3	0.1	0.013	6
Bruun *et al.* (1937)	1	0.05		6
Burrell and Robertson (1915a)	3	0.1	$0.005p$	4
Burrell and Robertson (1915b)	1,3	0.1	$0.005p$	4
Burrell and Robertson (1915c)	3	0.1	$0.005p$	2
Burrell and Robertson (1916)	1,3	0.1	$0.005p$	2,3
Butcher *et al.* (1972)	1	0.1	$p<1100$:1.4, $p>1100$:3.4	7
Calado and Soares (1977)	1	0.01	1	1
Calado *et al.* (1974)	1	0.01	0.01	1
Calado *et al.* (1983)	1	0.1		2
Calingaert *et al.* (1944)	16	0.01	0.013	8
Camin and Rossini (1955)	4	0.002 {0.008–0.015}		11,13–15
Camin *et al.* (1954)	4	0.002 {0.008–0.015}		16
Campbell *et al.* (1968)	1	0.01	0.0067	6
Campbell *et al.* (1986)	1	0.04 {0.1}	0.69 {0.69}	5
Carmichael *et al.* (1953)	1	0.011	$0.0025p$	9
Carmichael *et al.* (1962)	1	0.011	$0.001p$	4
Carruth and Kobayashi (1973)	8			2–10
Chaudhari and Katti (1990)	6	0.01	0.01	6–8
Cherney *et al.* (1949)	1	0.02	$0.0002p$ {$0.0025p$}	3
Chirico *et al.* (1989)	1,4	0.001	0.0001	10,20,28
Chui and Canfield (1971)	1	0.002	$0.0002p$	2
Chun (1964)	1	0.005 {0.1}	0.14 {0.69}	3,6
Clark (1973)		0.05 {0.05}	$p<3400$:$0.0001p$, $p>3400$:$0.0004p$ {$p<3400$: 0.28, $p>3400$:17}	3
Clark and Stead (1988)	6	[d]	$p<1100$:1, $p>1100$:6	2–4
Clegg and Rowlinson (1955)	1	0.01	4.1	3
Clusius *et al.* (1959)	1		0.013	1
Clusius *et al.* (1960)		0.01	0.0013	1

TABLE 3. Experimental methods used to determine vapor pressure, the precision and accuracy in temperature ΔT, the precision and accuracy in pressure Δp, and fluids studied—Continued

Author	Method[a]	ΔT/K[b]	Δp/kPa[b]	Fluids[c]
Connolly (1962)	1	0.01	1 {0.001p}	4
Cook (1958)	1		0.013	7,8
Cutler and Morrison (1965)	1	0.0002	0.0067	1
Dana *et al.* (1926)	1	0.03	0.003p {0.005p}	3,4
Dawson *et al.* (1973)	1	0.0001T	0.0004p	5
Day and Felsing (1951)	1	0.005	0.1	6
de Loos *et al.* (1988)	1	0.01	20	6,7
Dejoz *et al.* (1996)	6	0.1	0.01	8,10,12
Delaplace (1937)		0.56	0.000069 {0.05p}	2–4
Denig (1921)	1			6
Deschner and Brown (1940)	1			3
Diller *et al.* (1985)	3	0.02	4	5
Djordjevich and Budenholzer (1970)	6	0.056	$p<2.7$:0.04p, $2.7<p<100$:0.067, $100<p<690$: 0.69, $p>690$:6.9	2,3
Douslin (1970)	1			5,8
Douslin and Harrison (1973)	1	0.001	$<0.0001p$	2
Drucker *et al.* (1915)	3			6
Edgar *et al.* (1929)	3	0.5	0.013	7
Eggertsen *et al.* (1969)	8		0.045p	16
Elliot *et al.* (1974)	8	0.01	$p<2100$:2.1, $p>2100$:14	1,4
Eng and Sandler (1984)	7	0.001 {0.02}	0.0067 {0.021}	5,7
Enokido *et al.* (1969)				5
Escudero *et al.* (1992)	3	0.1	0.13	10
Eucken and Berger (1934)				1
Ewing and Goodwin (1991)	4	0.001	{0.0001p}	5
Ewing and Marsh (1973)	1	0.001 {0.01}	0.001 {0.01}	6
Fawcett (1946)	3	0.1		7
Felsing and Watson (1942)	1	0.01	0.0003p	8
Flebbe *et al.* (1982)	1	0.007	$p<667$:0.1, $p>667$:0.00015p	4
Forziati *et al.* (1949)	3	0.003	0.008	7,9
Francis and Robbins (1933)	1		0.0005p	3
Francis and Wood (1926)	3			16,22,24,26,28–30,34
Frank and Clusius (1939)				1
Fransson *et al.* (1992)	1	0.005	1.8 {0.015p}	5
Freeth and Verschoyle (1931)	1	0.1	1	1
Funk *et al.* (1972)	1	0.01	0.013	6–8
Gainar *et al.* (1992)	1	0.0005T	0.01p	4
Gehrig and Lentz (1983)				10
Genco *et al.* (1980)	1	0.01 {0.1}	2.7 {6.9}	6
Gierycz *et al.* (1985)	5	0.001 {0.002}	0.001 {0.003}	6,12
Gierycz *et al.* (1988)	5	0.001 {0.001}	0.0005 {0.003}	8,10
Gilliland and Scheeline (1940)	1	0.56	14	3,4
Glaser and Ruland (1957)				6
Grauso *et al.* (1977)	6	0.01	0.0002p	2,3
Gregorowicz *et al.* (1987)	5	0.01	0.0067	8,10
Grenier-Loustalot *et al.* (1981)	8	0.1	0.0013	16–22, 24–26, 28
Gugnoni *et al.* (1974)	1	0.01 {0.01}	0.69 {1.4}	2
Hachmuth (1932)	1	0.056		3–5
Harteck and Edse (1938)	1	0.01	0.013	3
Henning and Stock (1921)	1			1
Hestermans and White (1961)	1	0.01	$p<250$:0.0027, $p>250$:0.000 001p–0.000 03p	1
Hicks-Bruun and Bruun (1936)	3	0.05	0.0013	3
Higashi *et al.* (1994)	1	0.01	5	3,4
Hipkin (1966)	1,6			3,4
Hirata and Suda (1966)	1			4
Hirata *et al.* (1969)	1,6	0.1	5.1	2–4
Hlousek and Hala (1970)	3	0.01	0.0005p	7
Holcomb *et al.* (1995)	1	0.05	3.5	2–6
Holldorff and Knapp (1988)	1	0.04	0.001p+0.06 {$<0.005p$}	4
Hopfner *et al.* (1974)				5
Horner *et al.* (1975)	1			5
Howat and Swift (1985a)	1	0.03	0.08 {0.1}	5
Howat and Swift (1985b)	1	0.02	0.08 {0.002p}	5
Hsu *et al.* (1985)	1	0.56	5	4

TABLE 3. Experimental methods used to determine vapor pressure, the precision and accuracy in temperature ΔT, the precision and accuracy in pressure Δp, and fluids studied—Continued

Author	Method[a]	ΔT/K[b]	Δp/kPa[b]	Fluids[c]
Huckel and Rassmann (1933)				4
Huffman *et al.* (1961)		0.01	0.0013	7
Isaac *et al.* (1954)	1			5
Jansoone *et al.* (1970)	1	0.003 {0.02}	1	1
Kahre (1973)	1	0.056	3.4 {$0.001p-0.006p$}	2–4
Kahre (1974)	1	0.056	14	1
Kahre (1975)	1	0.056	14	1,5
Kay (1938)	1	0.01	$p<4100$:$0.0002p$, $p>4100$:6.9 {$0.005p$}	2,7
Kay (1940a)	1		$0.004p$	4
Kay (1940b)	1	0.056	$0.003p$	2,4
Kay (1941)	1	0.056	$0.003p$	4,7
Kay (1946)	1	1	4.1 {$0.004p$}	6
Kay (1970)	1	0.02 {0.5}	3.4 {14}	3–5
Kay (1971)	1	0.02 {0.5}	1.4 {14}	3,6,7
Kay and Warzel (1951)	1		0.069 {$0.0008p$}	8
Keistler and Van Winkle (1952)	6			12
Kemp and Egan (1938)				3
Keyes *et al.* (1922)	1	0.01		1
Khazanova *et al.* (1966)		0.05	5.1	2
Khurma *et al.* (1983)	1	0.02 {0.03}	$0.0001p$	5
Kilpatrick and Pitzer (1946)	2	0.01	0.0067	6
Kleinrahm and Wagner (1986)	1	0.003	larger of $0.000\,07p$ or 0.030	1
Kneisl and Zondlo (1987)	1	0.05	0.1	14
Kobe *et al.* (1955)	1	0.028	14	7
Kolasinska *et al.* (1982)	1	0.01	0.001	6–10
Krafft (1882a)	3			9–19
Krafft (1882b)	3			20–24,27
Krafft (1886)	3			31,32,35
Kratzke (1980)	1	0.01	$0.0003p$ {$0.0005p$}	3
Kratzke and Muller (1984)	1	0.01	$0.0001p$ {$0.001p$}	3
Kratzke *et al.* (1982)	1	0.002	$0.0003p$ {$0.05p-0.06p$}	4
Kratzke *et al.* (1985)	1	0.01	$0.001p$	5
Ksazczak (1989)	1	0.01	0.001	6
Kuenen and Robson (1902)	3	0.01	3 {30}	2
Laurance and Swift (1974)	1	0.0056	$0.001p$	4
Lee *et al.* (1992)	1	0.01	$p<100$:0.1, $p>100$:1	10,16
Leslie and Carr (1925)	3	0.05	0.2	6–8
Letcher and Marsicano (1974)	1	0.01	0.027	6
Leu and Robinson (1987a)	1	0.1	16	5
Leu and Robinson (1987b)	1	0.1	16	4
Leu and Robinson (1988)	1	0.1	16	5
Leu and Robinson (1989)	1	0.1	15	4
Lhotak and Wichterle (1981)	1	0.001 {0.01}	1	4
Li and Canjar (1953)	1		$0.001p$	5
Li *et al.* (1972)	1	0.01	0.0067	5,6
Li *et al.* (1973)	1	0.005	0.004	6
Linder (1931)	15		0.0027	8,10,14
Loomis and Walters (1926)	3	0.01	0.1	2
Maass and Wright (1921)	3	0.2	$0.0003p$	2,3
Machin and Golding (1989)	1	0.002	$p<1$:0.0003, $p>1$:$0.0006p$	4
Macknick and Prausnitz (1979)	8,13	0.05	$0.022p$	18,20
Mair (1932)	3	0.01	0.0013	5–10
Malewski and Sandler (1989)	6	0.05	0.69	4
Manley and Swift (1971)	1	0.01	1	3
Martin and Youings (1980)	12	0.001	0.008	6–8
Martinez-Ortiz and Manley (1978)	1	0.011	0.14 {$0.0004p$}	4
Mathews (1926)	3	0.05	0.013	7
Matuszak and Frey (1937)	3	1		4
Mazee (1948)	3			21,23,24,28,30,31,34–36,43
McGlashan and McKinnon (1977)	1	0.05	$0.0005p+0.3$	5
McMicking (1961)	1	0.001	$p<300$:0.13, $p>300$:0.53	7,8
McMicking and Kay (1965)	1	0.001 {0.05}	$p<300$:0.13, $p>300$:0.53 {3}	7,8
Mertes and Colburn (1947)	1,4	0.056	0.13	4
Messerly and Kennedy (1940)	1	0.01	0.0013	5

TABLE 3. Experimental methods used to determine vapor pressure, the precision and accuracy in temperature ΔT, the precision and accuracy in pressure Δp, and fluids studied—Continued

Author	Method[a]	ΔT/K[b]	Δp/kPa[b]	Fluids[c]
Meyer and Stec (1971)	3			24
Miksovsky and Wichterle (1975)	1	0.01	5.1	2,3
Milazzo (1956)		0.001 {0.01}	0.000 067	8
Millat *et al.* (1994)	1	$0.00005T$	0.015	8
Mills and Fenton (1987)	9	0.01	0.005	16
Miniovich and Sorina (1971)		0.002	0.49	2
Morecroft (1964)	9	0.02		19,27
Morgan and Kobayashi (1994)	1	0.03	$0.0015p+0.0048$	10,12,14,16,18–20,22,24,28
Mousa (1977)	1	0.2	3.4	3,6
Mundel (1913)				6–8
Myers and Fenske (1955)	3	0.2	$p<0.4$:0.0013, $0.013<p<4$:0.013, $p>4$:0.067	16,18,20
Neff and Hickman (1955)	3		$0.01p$	7,8
Neumann and Watch (1968)	1	0.05	4.9	1
Nicolini (1951)	1,6	0.05	0.0027	5,6,8
Niesen (1989)	1	0.05	3.5	4
Nunes da Ponte *et al.* (1985)	1	0.01 {0.1}	0.6 {1}	2
Ohgaki and Katayama (1977)	1	0.01	1	2
Olds *et al.* (1944)	1	0.0056	$0.001p$ {$0.002p$}	4
Olds *et al.* (1949)	1	0.056	$0.001p$	4
Olivares Fuentes *et al.* (1983)	3	0.04	0.0013	5,8
Olson (1995)	3	0.01	0.1 {$0.002p-0.005p$}	7
Ormandy and Craven (1923)	15	0.1	0.0013	7
Osborn and Douslin (1974)	1,4	0.001	$<0.001p$	5,7–9
Osborn and Scott (1980)	4	0.001	0.001	9
Oscarson *et al.* (1987)	3	0.1	$0.001p$ {$0.003p$}	6
Pal *et al.* (1976)	1	0.002 {0.015}	$0.0001p-0.0005p$	2
Palczewska-Tulinska *et al.* (1983)	3	0.005	0.02	7
Parks and Moore (1949)	9	0.1	$0.01p$	16
Parrish and Hiza (1974)	6	0.01	$p<690$:0.69, $p>690$:2	1
Piacente and Scardala (1990)	11	0.5	0.14	24–26,28
Piacente *et al.* (1991)	9,10,11	0.5		20–29
Piacente *et al.* (1994)	10			20–28,30–34,36–38
Porter (1926)	1	0.01	0.1	2
Prasad (1982)	1	0.01	$0.0001p$ {$0.005p$}	3
Prydz and Goodwin (1972)	1	0.006 to 0.016	$p<50$:0.02, $p>50$:$0.0004p$	1
Quitzsch *et al.* (1963)	16	0.02	$p<24$:0.0013, $p>24$:0.0027	7
Raal *et al.* (1972)	3,6	0.1	0.053	6,7
Reamer and Sage (1963)	1	0.056	1.4	10
Reamer *et al.* (1949)	1		$0.003p$	3
Reamer *et al.* (1951)	1	0.011	$p<2100$:2.1, $p>2100$:$0.001p$	3
Reamer *et al.* (1953)	1	0.017	$p<1400$:1.4, $p>1400$:$0.001p$	5
Regnier (1972)	3	0.1	$0.001p$	2
Richards and Hargreaves (1944)	3,6	0.05		7
Rogalsk *et al.* (1987)	3			10
Rotter and Knickle (1977)	3,6	0.1	0.27	6
Royo and Losa (1985)	1			6
Saez *et al.* (1985)	3	0.03	0.007	6,7
Sage and Lacey (1938)	1	0.056	1.4	4
Sage and Lacey (1942)	1	0.011	0.34 {$0.002p$}	5
Sage and Lacey (1948)	1	0.028	$0.003p$	4
Sage *et al.* (1934)	1	0.11	$p<2100$:0.69, $2100<p<21000$:6.9	3
Sage *et al.* (1937)	1	0.011	0.34 {1}	4
Sako *et al.* (1997)	1	0.03	0.3 {$0.0003p$}	4
Sasse *et al.* (1988)	1	0.02	$0.02p$	12,20,22,24
Schiessler and Whitmore (1955)	3,6	0.2 {0.5}		20
Schindler *et al.* (1966)	1	0.01	14	3
Schumann *et al.* (1942)	1			5
Seibert and Burrell (1915)	1	0.1	$0.005p$	4
Shealy and Sandler (1985)	7	0.001 {0.02}	0.02 {0.02}	7
Shepard *et al.* (1931)	3	0.01	1	5–12
Shibata and Sandler (1989)	6	0.05	0.69	4
Shim and Kohn (1962)	6	0.02		6
Silberberg (1958)	1	0.01	0.01 {$0.0025p$}	5
Silberberg *et al.* (1959)	1	$0.0002T$	$0.0004p$ {$0.0025p$}	5

TABLE 3. Experimental methods used to determine vapor pressure, the precision and accuracy in temperature ΔT, the precision and accuracy in pressure Δp, and fluids studied—Continued

Author	Method[a]	ΔT/K[b]	Δp/kPa[b]	Fluids[c]
Simons and Mausteller (1952)	3	0.01	0.13	4
Singh and Miller (1979)	1	0.01	$p<2000$:10, $p>2000$:100	1
Sinor *et al.* (1966)	1	0.02	10	1
Sipowska and Wieczorek (1980)	1	0.001	0.003	7
Sipowska and Wieczorek (1984)	1	0.001	0.003	7
Skripka *et al.* (1970)		0.01		1–4
Smith (1940)	5	0.001 {0.005}	0.0013	7,8
Smith (1941)	5	0.001 {0.01}		7,9
Smith and Matheson (1938)	5	0.001	0.0013	7,8
Smith and Robinson (1970)	1	0.02	0.0067 {0.04}	6
Smyth and Engel (1929)	3, 6	0.2	0.013	6,7
Stadnicki (1962a)	5	0.01		11
Stadnicki (1962b)				9
Stead and Williams (1980)	1	0.01	$p<1100$:1.4, $1100<p<4100$:6, $p>4100$:20	5
Steele *et al.* (1976)	1	0.017	0.069	4
Stock (1923)	1			1
Straty and Tsumura (1976)	1	0.003	$0.00015p$ {$0.0005p$}	2
Stryjek *et al.* (1974)	1	0.01	$0.01p$	2
Sunner and Svenson (1979)	2	0.01	0.001	13–15
Teichmann (1978)	1			3
Thomas and Harrison (1982)	1	0.0005	$p<10000$:0.0005, $p>10000$:0.002	3
Thomas and Young (1895)	1, 15	0.01	0.0067	6
Tickner and Lossing (1951)	14	0.3	$p<0.0013$:0.00013, $0.00\,13<p<1.3$:0.0013	2–5
Timrot and Pavlovich (1959)	16	0.01	{$0.0001p$}	1
Uchytil and Wichterle (1983)	1	0.01	0.5	3
Van Hook (1966)	1	0.01	0.0013	2
Van Itterbeek *et al.* (1963)	1	0.01	0.098	1
Van Itterbeek *et al.* (1964)	1	0.002	0.39	1
Van Ness *et al.* (1967)	1	0.01		7
Vennix *et al.* (1970)	1	0.01	$0.0001p$	1
Viton *et al.* (1996)	1	0.02	$p<0.67$:$0.02p$, $0.67<p<1.33$:$0.01p$, $1.33<p<40$: $0.003p$, $p>40$:$0.002p$	10–20
Wackher *et al.* (1945)	1	0.1 {0.1}	0.013 {$0.03p$}	4
Ward and Van Winkle (1954)	6		0.067	14
Waxman and Gallagher (1983)		0.002	$0.0001p$	4
Weber (1985)	1	0.02	0.2 {$0.0035p-0.019p$}	4
Weber (1989a)	1	0.01	3	4
Weber (1989b)	1	0.01	3	4
Weber (1999)	4	0.006	$0.0004p$ {$0.0005p-0.003p$}	7
Weiguo *et al.* (1990)	1	0.002	0.003 {0.01}	6,8
Weissman and Wood (1960)	6	0.01	0.011 {0.011}	8
Whitmore and Fleming (1933)	1	0.1	0.013	5
Whitmore *et al.* (1945)			$0.005p$	26
Wibaut *et al.* (1939)	3	0.05	0.0013 {$0.01p$}	5–9
Wichterle and Kobayashi (1972a)	1	0.01 {0.01}	$0.001p$ {$0.001p$}	1,2
Wichterle and Kobayashi (1972b)	1	0.01 {0.01}	$0.001p$ {$0.001p$}	1,3
Wieczorek and Stecki (1978)	1	0.001	0.0027	6
Willingham *et al.* (1945)	4	0.002	0.0053	5–10,12
Willman and Teja (1985)	7	0.2	0.13	10
Wisniewska *et al.* (1993)	3	0.01	0.05 {0.2}	7
Wojciechowski (1940)	5	0.002 {0.01}		6–9
Wolff and Hoeppel (1966)	1	0.02	0.13	6
Wolff and Hopfner (1965)	1			4,6
Wolff and Shadiakhy (1981)	1	0.02	0.03	6
Wolff and Wuertz (1968)	1			6
Wolff *et al.* (1964)	1			4,6,9
Wolff *et al.* (1980)	1	0.02	0.003	6
Woringer (1900)	1			6,8,10
Wu and Sandler (1988)	7	0.001 {0.02}	0.02 {0.02}	6
Wu *et al.* (1991a)	7	0.02	0.0013	8
Wu *et al.* (1991b)	7	0.001 {0.02}	0.02 {0.02}	8
Young (1897)	3	0.05	0.013	5
Young (1898)	1,3	0.01	0.0013	7
Young (1900)	1,3	0.05	0.0067	8

TABLE 3. Experimental methods used to determine vapor pressure, the precision and accuracy in temperature ΔT, the precision and accuracy in pressure Δp, and fluids studied—Continued

Author	Method[a]	ΔT/K[b]	Δp/kPa[b]	Fluids[c]
Young (1928)	3	0.028	0.013	1–8,20–35
Zanolini (1964)	1	0.11	$p<210$:0.069, $210<p<690$:1.4, $p>690$:4.1	3,5
Zawisza and Vejrosta (1982)	1	0.01	1 {2}	7
Zielkiewicz (1991)	1	0.02	0.004 {0.02}	6,7
Zielkiewicz (1992)	1	0.002	0.004 {0.02}	7,8
Zielkiewicz (1993)	1	0.002	0.004 {0.02}	7

[a] 1: Static, 2: Calorimetry static, 3: Ebulliometry, 4: Comparative ebulliometry, 5: Comparative Swietoslawski ebulliometer, 6: Recirculating still, 7: Stage–Muller recirculating still, 8: Gas saturation, 9: Knudsen effusion, 10: Torsion effusion, 11: Transpiration, 12: Continuous dilution, 13: Infrared detection, 14: Mass spectroscopy, 15: Ramsey–Young method, 16: Tensimeter.

[b] The accuracy, if cited by the authors, is provided in brackets.

[c] Numbers given are the number of carbon atoms in the molecule.

[d] $T<273$ K: 0.008 K; $T>273$ K: 0.01 K.

critical pressure, and ω listed in Table 2 were used as the basis for a new equation to represent the vapor pressures of normal alkanes C_nH_{2n+2} with $n\leqslant 36$ from the triple point, T^{s+1+g}, to the critical point. Although experimental data are available for $C_{37}H_{76}$, $C_{38}H_{78}$, and $C_{43}H_{88}$, they were not useful in the accuracy assessment of the equation due to the large uncertainties in these data. The temperatures at the normal boiling point determined from Eq. (12) are also listed in Table 2. Values of the triple point temperature are reported by Morgan and Kobayashi (1991). The critical temperatures reported in Table 2 were taken from the references cited in this table for the lower alkanes up to n-octane and were obtained from Eq. (20) for n-nonane and above. Values of the critical pressures in Table 2 were also taken from the literature for methane and ethane, determined in the regression analysis described below for propane through n-octane, and were obtained from Eq. (21) for n-nonane and above.

The vapor pressure measurements included in the preliminary analysis were selected from the database summarized in Table 4 on the basis of sample purity and of the uncertainty in vapor pressure calculated from Eq. (22). This uncertainty was based on the precision in temperature and pressure cited by the authors and listed in Table 3. Adjustments were made to this initial selection based on agreement between different data sets and deviations of the data sets from this and other correlations. The data sets used in the final regression are identified in Table 4. The coefficients of the generalized vapor pressure correlation presented here, N_1 through N_{12} in Eq. (12), are listed in Table 5 and were determined by nonlinear regression to the selected n-alkane data sets. The values of ω for ethane, propane, n-butane, and fluids with $n\geqslant 6$ and the critical pressures for propane through n-octane were fitted simultaneously with the N_i coefficients in the nonlinear regression to optimize the representation of the vapor pressure data with Eq. (12). The fitted critical pressures agree with those recommended by Ambrose and Tsonopoulos within the experimental uncertainties reported by them. For most n-alkanes with $n\geqslant 9$, measured vapor pressures do not extend to temperatures near the critical point and, consequently, the critical pressures were estimated from Eq. (21) and are listed in Table 2.

The values of ω for methane and n-pentane were constrained to the acentric factor ϖ given in Eq. (23), using vapor pressure equations from Setzmann and Wagner (1991) for methane and Kratzke *et al.* (1985) for n-pentane:

$$\varpi=\left(-\log\frac{p^{1+g}}{p_c}-1\right)_{T=0.7T_c}. \tag{23}$$

The vapor pressure p^{1+g} is determined at $0.7\cdot T_c$. A quadratic function of n was sufficient to adequately represent ω over the entire range for which vapor pressure measurements are available. However, in order to improve the extrapolation for the correlation for $n>50$, the following empirically determined functional form for ω, which has a limiting value of c_1, was adopted:

$$\omega=c_1-\exp(c_2+c_3n^{c_4}). \tag{24}$$

The coefficients c_2, c_3, and c_4 were simultaneously optimized during the nonlinear fitting process with the other parameters discussed above and are listed in Table 1. During the optimization of the coefficients, the upper limit of ω (the coefficient c_1) was selected as 3 to reproduce reasonable vapor pressures at $n>50$. The values of ω for $n\geqslant 8$ listed in Table 2 were calculated from Eq. (24). The values of ω determined this way are not reproduced exactly by Eq. (23) when Eq. (12) is used to calculate the vapor pressures.

Only vapor pressure data for the n-alkanes from methane to n-decane and fluids with carbon numbers divisible by 4 from n-dodecane to n-octacosane were used in determining the coefficients of Eq. (12). Data for the other fluids were not used since the uncertainties for these data sets were higher, and the available data did not span a significant fraction of the fluid range.

In order to obtain reasonable extrapolation behavior for the vapor pressure correlation at high ($n>100$) carbon numbers, constraints were placed on the functional form. The extrapolation of Eq. (20) for T_c and Eq. (12) for $T^{1+g}(101.325\,\mathrm{kPa})$ and $T^{1+g}(1\,\mathrm{kPa})$ are shown in Fig. 3 as a function of n, along with values recommended from TRC (Thermodynamic Research Center, 1997). At $n=100$, values reported by TRC agree within $0.013\cdot T^{1+g}$ at 0.101 325 MPa and within $0.04\cdot T^{1+g}$ at 1 kPa of our equation. Equation (12) gives limiting values ($n\to\infty$) of T(101.325 kPa) $=1117$ K and T(1 kPa)$=986$ K.

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties		Purity (mole fraction)	AAD (%)
				$100\Delta p/p$ at $T_{\min}$	$100\Delta p/p$ at $T_{\max}$		
Methane							
Armstrong *et al.* (1955)	100	91–190	12–4500	0.17	0.031		0.17
Bloomer and Parent (1953)	20	105–191	58–4610	0.79	0.17	0.9997	0.41
Calado and Soares (1977)	2	104–116	51–140	2	0.72	0.999	0.22
Calado *et al.* (1974)	2	116–135	140–487	0.077	0.056	0.999	0.082
Clusius *et al.* (1959)	6	110–111	85–96				0.069
Clusius *et al.* (1960)	9	91–98	12–27	0.13	0.11		0.11
Cutler and Morrison (1965)	15	93–108	16–73	0.042	0.0093	0.9998	0.31
Elliot *et al.* (1974)	6	144–191	793–4630	0.27	0.32	0.9997	0.59
Eucken and Berger (1934)	28	132–190	402–4620				3.2
Frank and Clusius (1939)	16	99–100	31–35				0.092
Freeth and Verschoyle (1931)	2	91	12	8.8	8.8		0.22
Henning and Stock (1921)	22	91–112	12–104				0.5
Hestermans and White (1961)	18	109–190	86–4450	0.084	0.031	0.9996	0.4
Jansoone *et al.* (1970)	7	190	4500–4580	0.024	0.024	0.9999	0.03
Kahre (1974)	3	166–186	2050–3990	0.7	0.39	0.9998	0.31
Kahre (1975)	2	178–186	3040–3990	0.49	0.39	0.9998	0.19
Keyes *et al.* (1922)	52	97–191	26–4670				1.2
Kleinrahm and Wagner (1986)	**161**	**91–191**	**12–4600**	**0.17**	**0.012**	**0.999 995**	**0.007**
Neumann and Watch (1968)	4	173–186	2640–4030	0.25	0.2	0.9995	0.68
Parrish and Hiza (1974)	6	95–120	20–192	3.5	1		0.24
Prydz and Goodwin (1972)	105	91–190	12–4520	0.18	0.064	0.9999	0.13
Singh and Miller (1979)	3	100–115	35–133	29	7.5	0.9997	0.81
Sinor *et al.* (1966)	6	93–188	21–4270	50	0.25	0.99	6.5
Skripka *et al.* (1970)	4	123–153	238–1190				0.13
Stock (1923)	35	89–123	9.5–229				1.3
Timrot and Pavlovich (1959)	9	112–191	101–4630				1.5
Van Itterbeek *et al.* (1963)	24	112–191	101–4640	0.13	0.032		0.9
Van Itterbeek *et al.* (1964)	38	112–190	111–4560	0.35	0.011		0.77
Vennix *et al.* (1970)	32	134–191	455–4610	0.058	0.077	>0.9999	0.18
Wichterle and Kobayashi (1972a)	8	130–191	372–4630	0.12	0.1	0.9997	0.49
Wichterle and Kobayashi (1972b)	7	130–191	372–4630	0.12	0.1	0.9997	0.63
Young (1928)	11	92–174	13–2660	0.36	0.096		0.73
Ethane							
Barclay *et al.* (1982)	7	198–278	200–2690	0.14	0.032	0.9996	0.2
Beattie *et al.* (1935a)	2	273–298	2390–4190	0.05	0.05	0.999	0.096
Brown *et al.* (1988)	8	207–270	294–2212	0.25	0.78	0.9999	0.18
Burrell and Robertson (1915c)	19	113–184	0.13–101	1.6	0.72		8.5
Burrell and Robertson (1916)	19	113–184	0.13–101	1.6	0.72		8.8
Carruth and Kobayashi (1973)	11	91–144	0.0015–5.7			0.9999	2.7
Chui and Canfield (1971)	2	116–161	0.68–24	0.022	0.025	0.9999[c]	36
Clark and Stead (1988)	3	260–280	1699–2791	0.35	0.22	0.99[c]	0.62
Delaplace (1937)	15	91–105	0.0033–0.095	6.3	3.4		50
Djordjevich and Budenholzer (1970)	6	128–255	1–1500	6.6	0.48	0.999	1.4
Douslin and Harrison (1973)	**18**	**238–305**	**913–4860**	**0.01**	**0.01**	**0.999 99**	**0.076**
Grauso *et al.* (1977)	4	200–290	218–3510	0.049	0.03	0.9995	0.13
Gugnoni *et al.* (1974)	4	241–283	1010–3010	0.075	0.032	0.9999	0.28
Hirata *et al.* (1969)	5	197–273	188–2340	2.7	0.33	0.98	1.6
Holcomb *et al.* (1995)	6	242–299	1036–4307	0.37	0.13		0.27
Kahre (1973)	5	267–300	2080–4300	0.22	0.14	0.9975	0.53
Kay (1938)	8	273–305	2410–4830	0.031	0.14	>0.97	0.29
Kay (1940b)	7	229–305	689–4830	0.35	0.32		0.55
Khazanova *et al.* (1966)	4	283–293	3070–3730	0.2	0.17		1.2
Kuenen and Robson (1902)	15	195–273	185–2430	1.6	0.13		1.6
Loomis and Walters (1926)	34	136–200	2.5–217	4.1	0.065		0.34
Maass and Wright (1921)	7	172–200	49–221	1.3	0.91		2
Miksovsky and Wichterle (1975)	2	303–305	4660–4800	0.11	0.11	0.9997	0.16
Miniovich and Sorina (1971)	16	303–305	4630–4870	0.011	0.011	0.9996	0.048
Nunes da Ponte *et al.* (1985)	8	210–284	331–3098	0.19	0.03	0.9999	0.24
Ohgaki and Katayama (1977)	5	283–298	3040–4210	0.04	0.032	0.997	0.72
Pal *et al.* (1976)	50	214–305	397–4850	0.031	0.03	0.9995	0.077

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

				Uncertainties			
Author[a]	No. of points	Temp. range K	Pressure range (kPa)	$100\Delta p/p$ at $T_{\min}$	$100\Delta p/p$ at $T_{\max}$	Purity (mole fraction)	AAD (%)
Porter (1926)	20	185–288	101–3390	0.11	0.022		0.23
Regnier (1972)	10	90–135	0.0013–2.3	2.3	1.1	0.999	6.9
Skripka *et al.* (1970)	5	203–273	249–2390				0.2
Straty and Tsumura (1976)	**43**	**160–300**	**22–4350**	**0.027**	**0.016**	**0.9998**	**0.043**
Stryjek *et al.* (1974)	4	139–194	3.4–175	1	1	0.9999	2.5
Tickner and Lossing (1951)	10	91–131	0.0013–1.3	13	3.7	0.997	16
Van Hook (1966)	182	112–201	0.11–224	1.2	0.045	>0.997	0.38
Wichterle and Kobayashi (1972a)	9	130–200	1.3–217	0.16	0.11	0.9999	0.74
Young (1928)	15	130–278	1.5–2660	0.96	0.065		1
Propane							
Barber (1968)	29	329–370	1940–4230	0.15	0.1	0.999	0.47
Beattie *et al.* (1935b)	17	323–348	1710–2850	0.032	0.031	0.999	0.041
Burrell and Robertson (1916)	16	149–229	0.4–101	0.91	0.65		18
Carruth and Kobayashi (1973)	12	98–179	0.000 006 6–4.6			0.9999	15
Cherney *et al.* (1949)	2	303–323	1080–1720	0.053	0.048	0.9999	0.19
Chun (1964)	10	348–367	2850–4090	0.011	0.0096	0.9999	0.62
Clark (1973)	10	327–370	1880–4210			0.9997	0.5
Clark and Stead (1988)	3	260–280	314–586	0.32	0.17	0.99[c]	0.86
Clegg and Rowlinson (1955)	9	323–370	1720–4250	0.24	0.097	0.9999	0.21
Dana *et al.* (1926)	43	210–323	37–1710	0.34	0.31	>0.995	0.55
Delaplace (1937)	27	90–126	0.000 034–0.01	[b]	8.8		41
Deschner and Brown (1940)	36	302–370	1050–4260			0.9827	1
Djordjevich and Budenholzer (1970)	6	128–255	0.013–259	[b]	2.7	0.9999	6.1
Francis and Robbins (1933)	34	301–337	1050–2400			0.99954	4.8
Gilliland and Scheeline (1940)	5	315–372	1410–4390	1.6	1.1	0.999	1.1
Grauso *et al.* (1977)	2	260–290	310–769	0.039	0.034	0.9995	0.12
Harteck and Edse (1938)	145	163–232	1.2–107	1.1	0.045		0.58
Higashi *et al.* (1994)	8	283–313	644–1380	0.77	0.36	0.99	0.9
Hipkin (1966)	4	267–366	385–3920			0.995	1.3
Hirata *et al.* (1969)	5	197–273	16–476	31	1.1	0.9985	0.89
Holcomb *et al.* (1995)	19	240–364	149–3792	2.4	0.13		0.24
Kahre (1973)	5	278–328	548–1880	0.65	0.22	0.998	0.55
Kay (1970)	10	332–368	2070–4140	0.17	0.091	0.999	0.41
Kay (1971)	9	332–390	2070–4830	0.078	0.049	0.995	0.44
Kemp and Egan (1938)	12	166–231	1.5–103			0.99998	0.91
Kratzke (1980)	**14**	**312–368**	**1330–4070**	**0.038**	**0.035**	**0.999 54**	**0.034**
Kratzke and Muller (1984)	5	300–357	1010–3360	0.027	0.021	0.99954	0.024
Maass and Wright (1921)	6	230–250	114–269	0.75	0.6		15
Manley and Swift (1971)	5	244–311	176–1300	0.57	0.081		0.15
Miksovsky and Wichterle (1975)	6	303–369	1080–4190	0.47	0.12	0.999	0.29
Mousa (1977)	11	335–370	2200–4250	0.43	0.37	>0.999	0.52
Prasad (1982)	14	298–368	941–4070	0.028	0.021	0.9999	1.8
Reamer *et al.* (1949)	10	313–370	1380–4260			0.999	0.32
Reamer *et al.* (1951)	6	278–361	545–3620	0.38	0.1	0.999	0.2
Sage *et al.* (1934)	21	294–371	862–4310	0.3	0.26		0.5
Schindler *et al.* (1966)	8	173–348	6.9–2900	[b]	0.48	0.9996	10
Skripka *et al.* (1970)	10	123–273	0.0049–472				5
Teichmann (1978)	15	325–363	1770–3780			0.9995	0.042
Thomas and Harrison (1982)	**25**	**258–370**	**292–4250**	**0.0017**	**0.000 91**	**0.999 98**	**0.028**
Tickner and Lossing (1951)	13	105–165	0.000 13–1.3	100	3		6.9
Uchytil and Wichterle (1983)	32	296–368	893–4120	0.062	0.022	0.9999	0.18
Wichterle and Kobayashi (1972b)	9	130–214	0.018–44	0.2	0.11	0.9999	3.5
Young (1928)	12	161–312	1.5–1330	0.93	0.065		11
Zanolini (1964)	13	273–347	475–2790	0.34	0.26	0.999	0.37
***n*-Butane**							
Aston and Messerly (1940)	11	195–273	1.3–102	0.1	0.0077		5.8
Beattie *et al.* (1939)	4	348–423	908–3670	0.006	0.0021		0.22
Brown *et al.* (1989)	2	250–270	40–92	1.8	0.77	0.999	0.45
Burrell and Robertson (1915a)	17	173–273	0.13–101	1.4	0.63		12
Carmichael *et al.* (1962)	26	311–380	355–1760	0.1	0.1	0.9991	0.37
Carruth and Kobayashi (1973)	14	135–213	0.0009–4.9			0.9993	5.6
Clark and Stead (1988)	3	260–280	61–134	1.6	0.75	0.99[c]	0.9

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

				Uncertainties			
Author^{a}	No. of points	Temp. range K	Pressure range (kPa)	$100\Delta p/p$ at $T_{\min}$	$100\Delta p/p$ at $T_{\max}$	Purity (mole fraction)	AAD (%)
Connolly (1962)	7	344–425	831–3780	0.12	0.031	0.9999	0.068
Dana *et al.* (1926)	19	255–331	50–605	0.33	0.31	>0.995	0.82
Delaplace (1937)	17	135–151	0.0009–0.01	11	8		7.9
Elliot *et al.* (1974)	13	144–278	0.0034–122	^{b}	11	0.9993	1.5
Flebbe *et al.* (1982)	12	278–358	125–1130	0.084	0.021	0.9995^{c}	0.056
Gainar *et al.* (1992)	12	300–353	258–1010	1.1	1		0.8
Hirata and Suda (1966)	25	333–401	640–2550			0.998	0.12
Hirata *et al.* (1969)	5	237–374	21–1540	24	0.38	0.995	0.2
Holcomb *et al.* (1995)	22	250–410	42–2943	8.3	0.15		0.88
Holldorff and Knapp (1988)	20	259–357	58–1100	0.27	0.14	0.9995	0.1
Hsu *et al.* (1985)	3	319–378	448–1660	1.9	1.1	0.9998	0.2
Kahre (1973)	2	289–328	179–545	1.9	0.65	0.999	1.1
Kahre (1974)	8	166–283	0.069–149	^{b}	9.3		2.6
Kay (1940a)	20	325–425	517–3790				0.27
Kay (1940b)	5	336–419	689–3450	0.33	0.31	>0.994	0.15
Kay (1941)	6	336–425	689–3790	0.33	0.31	>0.994	0.22
Kay (1970)	4	389–425	2070–3790	0.17	0.11	0.999	0.21
Kratzke *et al.* (1982)	**12**	**320–423**	**457–3662**	**0.03**	**0.03**	**0.999 52**	**0.036**
Laurance and Swift (1974)	3	311–339	355–734	0.1	0.1	0.9997	0.38
Leu and Robinson (1987b)	3	368–418	1386–3316	1.1	0.5	0.999	0.79
Leu and Robinson (1989)	6	366–418	1351–3344	1.1	0.48	0.999	1.5
Lhotak and Wichterle (1981)	15	293–363	208–1250	0.48	0.08	0.9996	0.12
Machin and Golding (1989)	**195**	**173–280**	**0.16–133**	**0.19**	**0.06**	**0.9995**	**0.042**
Malewski and Sandler (1989)	3	340–380	745–1758	0.15	0.1		0.75
Martinez-Ortiz and Manley (1978)	12	278–344	122–830	0.12	0.03	0.9999^{c}	0.05
Mertes and Colburn (1947)	8	293–394	206–2290	0.19	0.097	>0.99	0.87
Niesen (1989)	3	311–395	357–2259	0.99	0.18	0.9999	0.29
Olds *et al.* (1944)	4	311–411	355–3010	0.1	0.1	0.997	0.15
Olds *et al.* (1949)	4	311–411	355–3010	0.19	0.14	0.999	0.15
Sage and Lacey (1948)	4	311–411	355–3010	0.31	0.3	0.997	0.15
Sage *et al.* (1937)	7	294–394	216–2280	0.16	0.025	0.997	0.53
Sako *et al.* (1997)	22	301–316	265–405	0.15	0.11	0.9996	0.12
Seibert and Burrell (1915)	10	303–403	340–2790	0.56	0.53		11
Shibata and Sandler (1989)	3	311–411	356–3014	0.24	0.086		0.57
Simons and Mausteller (1952)	5	233–260	17–61	0.79	0.22	0.998	0.43
Skripka *et al.* (1970)	3	253–273	45–103				0.22
Tickner and Lossing (1951)	11	136–196	0.000 67–1.3	21	2.6		19
Wackher *et al.* (1945)	10	205–279	3.1–127	0.8	0.36	>0.99	3.7
Weber (1985)	4	250–280	39–132	0.52	0.17		0.2
Weber (1989a)	6	311–400	354–2493	0.84	0.12	>0.9994	0.25
Weber (1989b)	4	309–394	336–2252	0.89	0.13	>0.9994	0.29
Wolff and Hopfner (1965)	5	218–293	6.9–207				0.36
Wolff *et al.* (1964)	10	218–293	6.9–207				0.31
Young (1928)	15	194–403	1.5–2660	0.93	0.047		6.2
2-Methylpropane							
Aston *et al.* (1940)	9	188–262	1.5–102	0.088	0.0041		0.36
Beattie *et al.* (1949)	5	303–398	399–3080	2.9	1.7		0.51
Besserer and Robinson (1973b)	4	311–394	503–3020	0.31	0.1	0.999	3.5
Besserer and Robinson (1975a)	4	278–378	182–2160	11	0.96	0.999	0.55
Burrell and Robertson (1915b)	15	158–260	0.13–101	0.85	0.62		31
Carmichael *et al.* (1962)	26	311–380	496–2270	0.1	0.1	0.9994	0.4
Connolly (1962)	6	344–408	1110–3630	0.093	0.033	0.9996	0.083
Dana *et al.* (1926)	20	249–353	62–1340	0.33	0.31	>0.995	1.2
Delaplace (1937)	27	114–143	0.000 069–0.01	100	7.5		30
Gilliland and Scheeline (1940)	5	352–408	1370–3690	1.5	1	0.995	2.1
Hachmuth (1932)	5	273–289	159–265				0.86
Higashi *et al.* (1994)	5	283–313	228–527	2.2	0.95	0.99	2.1
Hipkin (1966)	5	267–394	123–2940			0.995	1.1
Hirata and Suda (1966)	29	295–374	317–2020			0.995	0.48
Hirata *et al.* (1969)	5	237–374	35–2020	14	0.31	0.9928	0.29
Huckel and Rassmann (1933)	46	220–263	15–110				3.6

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties $100\Delta p/p$ at $T_{\min}$	 $100\Delta p/p$ at $T_{\max}$	Purity (mole fraction)	AAD (%)
Kahre (1973)	5	278–328	186–758	1.9	0.47	0.9975	1.2
Leu and Robinson (1987b)	2	383–398	2456–3172	0.65	0.52	0.995	2.7
Leu and Robinson (1989)	6	344–398	1110–3054	1.4	0.52	0.995	0.45
Martinez-Ortiz and Manley (1978)	**10**	**278–344**	**183–1110**	**0.084**	**0.027**	**0.9999**[c]	**0.054**
Mertes and Colburn (1947)	8	293–394	298–2920	0.18	0.095	>0.99	0.75
Sage and Lacey (1938)	7	294–394	310–2890	0.48	0.11	0.9997	0.49
Seibert and Burrell (1915)	10	303–393	453–2890	0.56	0.53		6.2
Skripka *et al.* (1970)	7	203–273	4.9–156				1.5
Steele *et al.* (1976)	10	278–344	183–1110	0.068	0.037	0.9999	0.14
Tickner and Lossing (1951)	13	122–187	0.000 13–1.3	100	2.7		20
Wackher *et al.* (1945)	9	206–263	6.4–107	0.38	0.19	>0.99	2.3
Waxman and Gallagher (1983)	**16**	**298–398**	**350–3090**	**0.012**	**0.011**	**0.9998**	**0.068**
Weber (1985)	4	250–280	64–198	0.32	0.12		0.52
Weber (1989a)	5	311–400	497–3183	0.6	0.096	>0.9994	0.26
Weber (1989b)	4	311–394	497–2893	0.6	0.11	>0.9994	0.24
***n*-Pentane**							
Beattie *et al.* (1951b)	6	373–470	593–3380	0.11	0.079	0.9985	0.11
Besserer and Robinson (1973a)	4	278–378	30–648	70	3.2	0.999	1.2
Campbell *et al.* (1986)	3	373–423	587–1570	0.15	0.083	0.9984	0.27
Carruth and Kobayashi (1973)	10	144–242	0.000 081–3.4			0.9990	14
Douslin (1970)	9	260–331	13–203				0.1
Fransson *et al.* (1992)	4	324–385	166–754	1.1	0.24	>0.99	1.1
Holcomb *et al.* (1995)	29	250–409	8–1232	44	0.3		0.91
Horner *et al.* (1975)	34	265–297	17–64			0.9998	0.33
Howat and Swift (1985a)	2	313–323	112–159	0.13	0.11	0.998	1.8
Howat and Swift (1985b)	32	303–328	82–187	0.12	0.073	0.998	0.11
Kahre (1975)	7	178–283	0.015–38	[b]	36	0.9999	10
Kay (1970)	2	438–456	2070–2760	0.17	0.13	0.999	0.44
Khurma *et al.* (1983)	3	298–398	68–1000	0.075	0.04	0.999	0.071
Kratzke *et al.* (1985)	**14**	**350–460**	**339–2910**	**0.1**	**0.1**	**0.9996**	**0.051**
Leu and Robinson (1987a)	3	408–463	1200–2992	1.3	0.54	0.994	1
Li and Canjar (1953)	2	423–448	1590–2420			0.9988	0.11
Li *et al.* (1972)	7	293–311	57–107	0.04	0.034		0.15
Messerly and Kennedy (1940)	13	208–298	0.41–68	0.34	0.037		0.55
Nicolini (1951)	13	273–303	25–82	0.23	0.18		0.17
Olivares Fuentes *et al.* (1983)	25	275–315	27–124	0.18	0.13		0.087
Osborn and Douslin (1974)	**15**	**269–341**	**20–270**	**0.1**	**0.1**	**0.9998**	**0.083**
Reamer *et al.* (1953)	6	278–444	30–2270	4.5	0.1	0.995	0.53
Sage and Lacey (1942)	5	311–444	108–2270	0.32	0.023		0.24
Tickner and Lossing (1951)	13	147–223	0.000 13–1.3	100	2.3	0.9985	20
Willingham *et al.* (1945)	9	286–310	43–104	0.015	0.0085	0.9986	0.15
Young (1897)	28	243–309	5.1–101	0.4	0.17		0.56
Young (1928)	15	224–455	1.5–2660	0.93	0.044		1
Zanolini (1964)	14	314–456	121–2750	0.37	0.23	0.9997	0.67
2-Methylbutane							
Aston and Schumann (1942)	27	187–222	0.099–2	0.81	0.04		4.1
Besserer and Robinson (1975b)	4	278–378	42–786	49	2.6		0.64
Diller *et al.* (1985)	10	400–460	1250–3370	0.32	0.12	0.9999	0.15
Ewing and Goodwin (1991)	**28**	**255–323**	**15–205**			**0.999 84**	**0.02**
Hachmuth (1932)	3	273–295	35–83				0.6
Holcomb *et al.* (1995)	28	233–407	7–1398	50	0.27		3.9
Isaac *et al.* (1954)	3	398–448	1200–2800			0.9989	0.73
Leu and Robinson (1987a)	3	408–453	1482–3013	1.1	0.54	0.99	1.7
Schumann *et al.* (1942)	13	217–295	1.5–83			0.999 95	0.18
Silberberg (1958)	12	323–423	205–1870	0.03	0.017		0.2
Silberberg *et al.* (1959)	6	323–448	205–2790	0.19	0.04		0.18
Willingham *et al.* (1945)	7	289–302	67–104	0.011	0.0086	0.9946	0.026
2,2-Dimethylpropane							
Aston and Messerly (1936)	7	258–283	38–102	0.0057	0.0038	0.9927	0.23
Beattie *et al.* (1951a)	9	323–434	356–3200			0.999 82	0.43
Dawson *et al.* (1973)	**19**	**343–433**	**586–3170**	**0.089**	**0.04**	**0.9996**	**0.4**

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties 100$\Delta p/p$ at $T_{\min}$	100$\Delta p/p$ at $T_{\max}$	Purity (mole fraction)	AAD (%)
Douslin (1970)	8	265–304	51–203				0.27
Enokido *et al.* (1969)	6	257–261	36–43			0.9952	0.29
Hopfner *et al.* (1974)	43	257–293	36–145				0.2
Leu and Robinson (1988)	5	313–423	283–2810	5.5	0.57	0.9986	4.9
McGlashan and McKinnon (1977)	3	373–413	1120–2290	0.13	0.1	0.9997	0.49
Osborn and Douslin (1974)	**10**	**268–313**	**58–270**	**0.1**	**0.1**	**0.9995**	**0.35**
Stead and Williams (1980)	5	260–300	43–184	3.3	11	0.9988	2.3
Whitmore and Fleming (1933)	6	257–283	38–101	0.43	0.36		2.2
***n*-Hexane**							
Bell *et al.* (1968)	2	298	20				0.032
Bich *et al.* (1992)	**39**	**295–351**	**17–134**	**0.087**	**0.0075**	**0.999 52**	**0.045**
Bissell and Williamson (1975)	5	298	20	0.12	0.12	0.999	0.12
Brown (1952)	19	310–342	32–101	0.04	0.031		0.15
Campbell *et al.* (1968)	12	298–342	20–101	0.055	0.032		1.4
Carruth and Kobayashi (1973)	12	178–265	0.0014–3.1			0.9995	11
Chun (1964)	25	373–503	230–2830	0.061	0.0088	0.9996	0.99
de Loos *et al.* (1988)	5	472–507	1770–3025	1.1	0.66	0.99	0.49
Denig (1921)	7	398–503	586–2760				12
Drucker *et al.* (1915)	23	174–270	0.0012–5.2				7
Genco *et al.* (1980)	22	383–507	314–3030	0.86	0.09	0.9996	0.61
Gierycz *et al.* (1985)	2	333–343	77–105	0.0036	0.0033	0.9999	0.2
Glaser and Ruland (1957)	16	342–498	101–2530				2.9
Kay (1946)	6	342–503	101–2800	5.1	1.5		0.57
Kay (1971)	2	482–501	2070–2760	0.073	0.058	0.995	0.061
Ksazczak (1989)	32	283–310	9.8–32	0.051	0.04	0.9995	0.22
Leslie and Carr (1925)	12	287–342	12–101	1.6	0.25		0.91
Letcher and Marsicano (1974)	8	300–321	22–50	0.13	0.064	0.999	0.063
Li *et al.* (1972)	9	301–336	23–85	0.051	0.034		0.18
Li *et al.* (1973)	12	274–298	6.2–20	0.07	0.029	0.9999	0.084
Mousa (1977)	10	485–508	2160–3030	0.34	0.31	>0.999	0.45
Mundel (1913)	8	207–226	0.044–0.27				2.7
Oscarson *et al.* (1987)	17	313–433	35–903	0.43	0.21	0.99	1.2
Saez *et al.* (1985)	6	313–338	37–90	0.12	0.097	0.999	0.083
Shim and Kohn (1962)	7	248–423	1.3–747			0.99	1.6
Smyth and Engel (1929)	4	303–333	24–76	0.85	0.67		1.4
Thomas and Young (1895)	51	243–342	0.96–101	0.7	0.032		1
Weiguo *et al.* (1990)	3	298–308	20–31	0.017	0.013	0.9999	0.08
Wieczorek and Stecki (1978)	10	298–343	20–104	0.014	0.004	0.9997	0.028
Willingham *et al.* (1945)	16	286–343	12–104	0.047	0.0081	0.9991	0.036
Wolff and Hoeppel (1966)	5	223–293	0.29–16	45	0.83	0.9996	8.8
Wolff and Hopfner (1965)	9	218–293	0.13–16				3.4
Wolff and Shadiakhy (1981)	9	293–373	16–245	0.21	0.053	0.99979	0.16
Wolff and Wuertz (1968)	5	223–293	0.24–16			0.9996	5.1
Wolff *et al.* (1964)	7	233–293	0.49–16				2
Wolff *et al.* (1980)	8	223–293	0.24–16	1.3	0.21	0.997	4.5
Woringer (1900)	15	273–343	6.2–106				0.91
Wu and Sandler (1988)	8	307–339	30–93	0.067	0.022	0.999	0.062
Young (1928)	15	249–500	1.5–2660	0.93	0.041		1
2-Methylpentane							
Abara *et al.* (1988)	4	491–497	2771–2983	0.47	0.44	0.9995	0.12
Bruun and Hicks-Bruun (1930)	2	334	101	0.32	0.32		0.9
Chun (1964)	26	348–493	159–2830	0.088	0.0089	0.9970	0.72
Funk *et al.* (1972)	3	283–323	15–72	0.1	0.039	0.999	0.044
Holcomb *et al.* (1995)	30	239–408	1–675	[b]	0.53		3.7
Willingham *et al.* (1945)	**14**	**286–334**	17–104	**0.033**	**0.0082**	**0.9989**	**0.13**
3-Methylpentane							
Bruun and Hicks-Bruun (1930)	2	336	101	0.31	0.32		0.16
Chun (1964)	26	348–493	145–2660	0.096	0.0089	0.9983	0.79
Day and Felsing (1951)	5	423–504	831–3100	0.016	0.008	0.998	0.45
Funk *et al.* (1972)	3	283–323	13–65	0.11	0.04	0.999	0.054
Willingham *et al.* (1945)	**14**	**288–337**	**17–104**	**0.033**	**0.0081**	**0.9985**	**0.072**

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum T_{min} and maximum T_{max} temperature of the measurements—Continued

				Uncertainties			
Author[a]	No. of points	Temp. range K	Pressure range (kPa)	100$\Delta p/p$ at T_{min}	100$\Delta p/p$ at T_{max}	Purity (mole fraction)	AAD (%)
2,2-Dimethylbutane							
Chun (1964)	24	348–483	213–2840	0.066	0.0088	0.9999	0.88
Funk *et al.* (1972)	3	283–323	23–102	0.072	0.035	0.97	0.081
Kilpatrick and Pitzer (1946)	11	211–289	0.25–30	2.6	0.047	0.99995	1.4
Nicolini (1951)	19	27–3318	15–87	0.24	0.17		0.24
Willingham *et al.* (1945)	**11**	**289–324**	**29–104**	**0.02**	**0.0082**	**0.9994**	**0.02**
2,3-Dimethylbutane							
Bruun and Hicks-Bruun (1930)	2	331	101	0.32	0.32		0.67
Chun (1964)	26	348–493	168–2850	0.083	0.0087	0.9981	0.42
Ewing and Marsh (1973)	3	288–313	21–55	0.0065	0.004	0.9998	0.09
Funk *et al.* (1972)	3	283–323	16–78	0.093	0.038	0.97	0.062
Kay (1946)	6	331–493	101–2840	5.1	1.5		0.53
Willingham *et al.* (1945)	**13**	**287–332**	**20–104**	**0.028**	**0.0081**	**0.9990**	**0.094**
***n*-Heptane**							
Beattie and Kay (1937)	37	540	2730–2750				0.29
Bell *et al.* (1968)	2	298	6.1				0.082
Bissell and Williamson (1975)	2	298	6–6.1	0.41	0.41	0.9978	0.9
Brown (1952)	8	313–372	12–101	0.046	0.029		0.031
Butcher *et al.* (1972)	8	383–488	137–1220	1	0.33		2.4
Carruth and Kobayashi (1973)	10	185–296	0.000 29–5.1			0.9992	5.5
Cook (1958)	3	273–308	1.5–9.8				0.78
de Loos *et al.* (1988)	6	499–540	1530–2750	1.3	0.73	0.99	1.8
Forziati *et al.* (1949)	20	299–372	6.4–104	0.19	0.014	0.9996	0.032
Funk *et al.* (1972)	3	313–353	12–57	0.12	0.041	0.999	0.1
Hlousek and Hala (1970)	17	302–372	7.3–101	0.069	0.058		0.14
Kay (1938)	9	372–532	101–2410	0.036	0.29	>0.97	0.65
Kay (1941)	3	454–521	689–2070	0.32	0.31	>0.994	0.85
Kay (1971)	2	519–539	2070–2760	0.072	0.057	0.995	2.5
Kobe *et al.* (1955)	22	422–539	386–2700	3.6	0.51	0.9994	2.5
Leslie and Carr (1925)	12	313–372	12–101	1.6	0.25		1.5
Mathews (1926)	9	333–372	27–101	0.2	0.15		1.2
McMicking (1961)	28	382–540	142–2740	0.094	0.02	0.9992	1.2
McMicking and Kay (1965)	19	372–540	101–2740	0.13	0.02	0.9992	0.24
Mundel (1913)	7	210–233	0.013–0.1				32
Neff and Hickman (1955)	3	323–333	19–28			0.9993	0.22
Olson (1995)	7	397–475	205–1030	0.055	0.019	0.999	0.62
Ormandy and Craven (1923)	9	233–273	0.04–1.6	3.8	0.6		23
Palczewska-Tulinska *et al.* (1983)	11	316–371	14–100	0.15	0.025	0.9994	0.13
Quitzsch *et al.* (1963)	4	293–323	4.7–19	0.11	0.083		0.21
Saez *et al.* (1985)	7	323–353	19–57	0.13	0.1	0.999	0.17
Shealy and Sandler (1985)	5	323–343	19–41	0.11	0.05	0.999	0.14
Sipowska and Wieczorek (1980)	6	278–303	2.1–7.8	0.14	0.039	0.999	0.17
Sipowska and Wieczorek (1984)	8	298–363	6.1–79	0.049	0.0049	0.999	0.12
Smith (1940)	16	313–403	12–232	0.012	0.0025		0.03
Smith and Matheson (1938)	17	367–376	87–115	0.0034	0.0031		0.006
Smyth and Engel (1929)	11	296–372	5.5–101	1	0.59		0.48
Weber (1999)	**59**	**335–503**	**30–1598**	**0.046**	**0.041**	**0.993**	**0.072**
Willingham *et al.* (1945)	40	299–372	6.4–104	0.085	0.0078	0.9988	0.041
Wisniewska *et al.* (1993)	14	400–471	217–943	0.034	0.018	0.999	0.14
Young (1898)	29	270–372	1.2–102	0.13	0.029		0.59
Young (1928)	15	272–538	1.5–2660	0.92	0.04		0.34
Zawisza and Vejrosta (1982)	10	423–523	373–2148	0.27	0.049	0.9999	0.24
2-Methylhexane							
Abara *et al.* (1988)	3	516–529	2254–2693	0.58	0.48	0.99	0.24
Forziati *et al.* (1949)	**20**	**292–364**	**6.4–104**	**0.19**	**0.015**	**0.9982**	**0.12**
Huffman *et al.* (1961)	8	273–318	2.3–21	0.082	0.041		0.056
McMicking (1961)	27	372–530	133–2730	0.1	0.02	0.9991	0.36
McMicking and Kay (1965)	18	363–530	101–2730	0.13	0.02	0.9991	0.2
3-Methylhexane							
Forziati *et al.* (1949)	**20**	**293–366**	**6.4–104**	**0.19**	**0.015**	**0.998**	**0.096**
Funk *et al.* (1972)	6	283–353	3.8–70	0.35	0.037	0.97	0.11
McMicking (1961)	19	379–535	156–2810	0.085	0.022	0.9980	0.94
McMicking and Kay (1965)	19	365–535	101–2810	0.13	0.02	0.9980	0.15

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

				Uncertainties			
Author[a]	No. of points	Temp. range K	Pressure range (kPa)	$100\Delta p/p$ at $T_{\min}$	$100\Delta p/p$ at $T_{\max}$	Purity (mole fraction)	AAD (%)
2,2-Dimethylpentane							
Fawcett (1946)	8	353–483	103–1590				0.91
Forziati *et al.* (1949)	**19**	**285–353**	**7.7–104**	**0.16**	**0.015**	**0.9981**	**0.093**
McMicking (1961)	19	362–520	139–2770	0.096	0.019	0.9981	0.61
McMicking and Kay (1965)	18	352–520	101–2770	0.13	0.019	0.9981	0.13
Willingham *et al.* (1945)	30	288–353	9–104	0.06	0.0079	0.9998	0.2
2,3-Dimethylpentane							
Forziati *et al.* (1949)	**20**	**291–364**	**6.4–104**	**0.19**	**0.014**	**0.9980**	**0.1**
McMicking (1961)	24	373–537	151–2910	0.088	0.02	0.9985	2.1
McMicking and Kay (1965)	20	363–537	101–2910	0.13	0.019	0.9985	0.15
Osborn and Douslin (1974)	15	209–278	0.015–3.3	0.1	0.1	0.998	1.8
2,4-Dimethylpentane							
Fawcett (1946)	8	353–483	99–1580			0.95	1.1
Forziati *et al.* (1949)	**19**	**287–354**	**7.7–104**	**0.16**	**0.015**	**0.9988**	**0.067**
McMicking (1961)	23	368–520	156–2740	0.086	0.02	0.9988	0.66
McMicking and Kay (1965)	18	354–520	101–2740	0.13	0.02	0.9988	0.35
Richards and Hargreaves (1944)	3	354	101				0.33
3,3-Dimethylpentane							
Forziati *et al.* (1949)	**19**	**287–360**	**6.4–104**	**0.19**	**0.014**	**0.9978**	**0.009**
McMicking (1961)	**31**	**361–536**	**108–2950**	**0.12**	**0.018**	**0.9996**	**0.31**
McMicking and Kay (1965)	**20**	**359–536**	**101–2950**	**0.13**	**0.018**	**0.9996**	**0.2**
Willingham *et al.* (1945)	29	287–360	6.4–104	0.084	0.0077	0.9983	0.053
2,2,3-Trimethylbutane							
Fawcett (1946)	8	353–483	98–1490			0.97	0.6
Forziati *et al.* (1949)	**19**	**286–355**	**7.7–104**	**0.16**	**0.014**	**0.999 82**	**0.043**
McMicking (1961)	29	382–531	219–2950	0.061	0.019	0.99991	0.22
McMicking and Kay (1965)	19	354–531	101–2950	0.13	0.02	0.99991	0.15
Smith (1941)	15	296–379	12–199				0.081
3-Ethylpentane							
Forziati *et al.* (1949)	**18**	**294–367**	**6.4–104**	**0.19**	**0.014**	**0.9994**	**0.073**
McMicking (1961)	25	374–541	125–2890	0.11	0.019	0.9994	0.17
McMicking and Kay (1965)	20	367–541	101–2890	0.13	0.019	0.9994	0.12
Smith (1941)	15	308–391	12–199				0.1
***n*-Octane**							
Bell *et al.* (1968)	2	298	1.9				0.18
Carruth and Kobayashi (1973)	10	217–297	0.0024–1.6			0.9985	7.4
Cook (1958)	3	273–308	0.36–3.2				3
Dejoz *et al.* (1996)	39	291–409	1.2–134	1	0.26	0.998[c]	0.1
Felsing and Watson (1942)	8	373–548	101–1860	0.034	0.033		7.2
Gierycz *et al.* (1988)	3	373–399	47–101	0.0034	0.0028	0.9995	0.088
Gregorowicz *et al.* (1987)	**15**	**359–393**	**29–86**	**0.043**	**0.03**	**0.9995**	**0.045**
Leslie and Carr (1925)	12	335–397	12–101	1.6	0.24		5
Linder (1931)	3	264–277	0.2–0.49				1.9
McMicking (1961)	26	413–569	153–2490	0.087	0.021	0.9995	0.69
McMicking and Kay (1965)	18	399–563	101–2300	0.13	0.023	0.9995	0.16
Millat *et al.* (1994)	**19**	**306–393**	**2.9–86**	**0.52**	**0.018**	**0.999 05**	**0.1**
Mundel (1913)	4	238–263	0.022–0.18				3.3
Weiguo *et al.* (1990)	2	298–303	1.9–2.5	0.16	0.12	0.99	0.2
Willingham *et al.* (1945)	29	326–400	7.7–104	0.07	0.0075	0.9996	0.09
Woringer (1900)	26	273–398	0.54–103				12
Wu *et al.* (1991b)	2	353–383	23–65	0.086	0.031	0.999	0.34
Young (1900)	40	270–398	0.3–97	2.3	0.14		1
Young (1928)	14	294–557	1.5–2110	0.92	0.039		0.41
2-Methylheptane							
Abara *et al.* (1988)	3	547–553	2084–2291	0.62	0.57	0.99	0.74
McMicking (1961)	**20**	**398–560**	**125–2480**	**0.11**	**0.022**	**0.9966**	**0.15**
McMicking and Kay (1965)	**19**	**391–560**	**101–2480**	**0.13**	**0.022**	**0.9966**	**0.036**
Osborn and Douslin (1974)	11	233–283	0.025–1.2	0.1	0.1	0.99969	1.6
Willingham *et al.* (1945)	**28**	**315–392**	**6.4–104**	**0.084**	**0.0076**	**0.9990**	**0.14**
3-Methylheptane							
McMicking (1961)	22	399–564	122–2550	0.11	0.022	0.9962	0.17

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{l+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties		Purity (mole fraction)	AAD (%)
				$100\Delta p/p$ at $T_{\min}$	$100\Delta p/p$ at $T_{\max}$		
McMicking and Kay (1965)	20	392–564	101–2550	0.13	0.023	0.9962	0.19
Neff and Hickman (1955)	8	298–353	2.6–29			0.98	0.29
Osborn and Douslin (1974)	11	238–288	0.037–1.5	0.1	0.1	0.999 73	0.72
Willingham *et al.* (1945)	**30**	**316–393**	**6.4–104**	**0.084**	**0.0076**	**0.9994**	**0.11**
4-Methylheptane							
McMicking (1961)	23	398–562	125–2540	0.11	0.023	0.9989	0.26
McMicking and Kay (1965)	19	391–562	101–2540	0.13	0.024	0.9989	0.15
Willingham *et al.* (1945)	**30**	**315–392**	**6.4–104**	**0.084**	**0.0076**	**0.9985**	**0.027**
2,2-Dimethylhexane							
McMicking (1961)	24	393–550	146–2530	0.091	0.023	0.9989	0.26
McMicking and Kay (1965)	20	380–550	101–2530	0.13	0.022	0.9989	0.081
Willingham *et al.* (1945)	**20**	**305–381**	**6.4–104**	**0.084**	**0.0076**	**0.9982**	**0.11**
2,3-Dimethylhexane							
McMicking (1961)	24	398–563	132–2630	0.1	0.02	0.9985	0.27
McMicking and Kay (1965)	20	389–563	101–2630	0.13	0.02	0.9985	0.17
Willingham *et al.* (1945)	**20**	**312–390**	**6.4–104**	**0.084**	**0.0076**	**0.953**	**0.12**
2,4-Dimethylhexane							
McMicking (1961)	23	382–553	102–2560	0.13	0.021	0.9975	0.25
McMicking and Kay (1965)	19	383–553	101–2560	0.13	0.021	0.9975	0.068
Willingham *et al.* (1945)	**20**	**307–383**	**6.4–104**	**0.084**	**0.0076**	**>0.98**	**0.029**
2,5-Dimethylhexane							
McMicking (1961)	20	398–550	158–2490	0.084	0.024	0.9997	0.21
McMicking and Kay (1965)	19	382–550	101–2490	0.13	0.024	0.9997	0.13
Willingham *et al.* (1945)	**20**	**307–383**	**6.4–104**	**0.084**	**0.0076**	**0.99**	**0.071**
3,3-Dimethylhexane							
McMicking (1961)	25	398–562	145–2650	0.092	0.02	0.9975	0.15
McMicking and Kay (1965)	19	385–562	101–2650	0.13	0.02	0.9975	0.15
Willingham *et al.* (1945)	**20**	**309–386**	**6.4–104**	**0.084**	**0.0075**	**0.995**	**0.072**
3,4-Dimethylhexane							
McMicking (1961)	23	399–569	125–2690	0.11	0.022	0.9975	0.2
McMicking and Kay (1965)	20	391–569	101–2690	0.13	0.021	0.9975	0.2
Willingham *et al.* (1945)	**20**	**314–392**	**6.4–104**	**0.084**	**0.0075**	**>0.98**	**0.07**
2,2,3-Trimethylpentane							
Brooks *et al.* (1939)	5	383	101				0.26
McMicking (1961)	25	399–563	154–2730	0.087	0.02	0.9968	0.13
McMicking and Kay (1965)	20	383–563	101–2730	0.13	0.02	0.9968	0.056
Willingham *et al.* (1945)	**20**	**306–384**	**6.3–104**	**0.085**	**0.0075**	**0.993**	**0.06**
2,2,4-Trimethylpentane							
Beattie and Edwards (1948)	5	423–523	346–1930				0.51
Cook (1958)	3	273–308	1.7–10				0.74
Funk *et al.* (1972)	3	313–353	13–57	0.11	0.04	0.999	0.05
Kay and Warzel (1951)	**23**	**372–544**	**101–2560**			**0.9987**	**0.12**
McMicking (1961)	32	383–544	142–2570	0.093	0.023	0.9995	0.94
McMicking and Kay (1965)	19	372–544	101–2570	0.13	0.024	0.9995	0.48
Milazzo (1956)	13	195–298	0.0016–6.7	4.1	0.0049		1.2
Nicolini (1951)	21	297–348	6.4–48	0.24	0.17		1.6
Olivares Fuentes *et al.* (1983)	21	323–364	20–79	0.16	0.12		0.15
Smith (1940)	16	312–405	12–232	0.012	0.0024		0.08
Smith and Matheson (1938)	16	367–377	88–115	0.0033	0.003		0.099
Weissman and Wood (1960)	5	308–348	10–48	0.11	0.04		0.079
Willingham *et al.* (1945)	**40**	**297–373**	**6.4–104**	**0.084**	**0.0076**	**0.9988**	**0.067**
Wu *et al.* (1991a)	11	267–333	1.1–29	0.18	0.074	0.999[c]	2.8
2,3,3-Trimethylpentane							
McMicking (1961)	24	398–574	133–2820	0.1	0.02	0.9979	0.16
McMicking and Kay (1965)	**21**	**388–574**	**101–2820**	**0.13**	**0.02**	**0.9979**	**0.14**
Willingham *et al.* (1945)	**20**	**310–389**	**6.4–104**	**0.084**	**0.0075**	**0.9941**	**0.24**
2,3,4-Trimethylpentane							
Douslin (1970)	7	325–414	13–203				0.16
McMicking (1961)	23	398–566	139–2730	0.096	0.02	0.9983	0.17
McMicking and Kay (1965)	20	387–566	101–2730	0.13	0.02	0.9983	0.21
Osborn and Douslin (1974)	12	223–278	0.015–1.2	0.1	0.1	0.9995	2.2
Willingham *et al.* (1945)	**20**	**310–388**	**6.4–104**	**0.084**	**0.0075**	**0.9984**	**0.14**

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties 100Δp/p at $T_{\min}$	100Δp/p at $T_{\max}$	Purity (mole fraction)	AAD (%)
2,2,3,3-Tetramethylbutane							
Calingaert *et al.* (1944)	**7**	**374–383**	**87–111**	**0.032**	**0.029**	**0.9996**	**0.11**
3-Ethylhexane							
McMicking (1961)	24	398–565	121–2610	0.11	0.02	0.9975	0.091
McMicking and Kay (1965)	20	392–565	101–2610	0.13	0.02	0.9975	0.073
Willingham *et al.* (1945)	**20**	**315–393**	**6.4–104**	**0.084**	**0.0076**	**>0.98**	0.048
2-Methyl-3-ethylpentane							
McMicking (1961)	27	398–567	131–2700	0.1	0.02	0.9978	0.13
McMicking and Kay (1965)	20	389–567	101–2700	0.13	0.02	0.9978	0.1
Willingham *et al.* (1945)	**20**	**312–390**	**6.4–104**	**0.084**	**0.0075**	**0.995**	**0.038**
3-Methyl-3-ethylpentane							
McMicking (1961)	24	398–577	121–2810	0.11	0.021	0.9993	0.38
McMicking and Kay (1965)	**21**	**391–577**	**101–2810**	**0.13**	**0.02**	**0.9993**	**0.5**
Willingham *et al.* (1945)	**20**	**313–392**	**6.4–104**	**0.084**	**0.0075**	**0.995**	**0.39**
***n*-Nonane**							
Carmichael *et al.* (1953)	13	311–511	1.2–657	0.26	0.25	0.996	0.49
Carruth and Kobayashi (1973)	10	220–308	0.000 76–0.72			0.9968	21
Forziati *et al.* (1949)	20	343–425	6.4–104	0.19	0.014	0.9994	0.071
Krafft (1882a)	6	313–423	1.5–101				6.2
Stadnicki (1962b)	4	401–424	53–101				0.8
Willingham *et al.* (1945)	**20**	**343–425**	**6.3–104**	**0.084**	**0.0074**	**>0.997**	**0.086**
Wolff *et al.* (1964)	3	253–293	0.027–0.45				18
2,2,3-Trimethylhexane							
Osborn and Douslin (1974)	**14**	**238–303**	**0.019–2**	**0.1**	**0.1**	**0.9975**	**0.25**
2,2,4-Trimethylhexane							
Osborn and Douslin (1974)	**14**	**238–303**	**0.031–2.8**	**0.1**	**0.1**	**0.9975**	**0.41**
2,2,5-Trimethylhexane							
Forziati *et al.* (1949)	**18**	**319–398**	**6.4–104**	**0.19**	**0.014**	**0.9986**	**0.15**
Osborn and Douslin (1974)	**14**	**238–303**	**0.03–2.9**	**0.1**	**0.1**	**0.9986**	**0.53**
2,4,4-Trimethylhexane							
Forziati *et al.* (1949)	**18**	**324–405**	**6.4–104**	**0.19**	**0.014**	**0.9973**	**0.12**
2,2,3,3-Tetramethylpentane							
Forziati *et al.* (1949)	**20**	**331–414**	**6.4–104**	**0.19**	**0.014**	**0.9987**	**0.12**
2,2,3,4-Tetramethylpentane							
Forziati *et al.* (1949)	**20**	**325–407**	**6.4–104**	**0.19**	**0.014**	**0.999 76**	**0.051**
2,2,4,4-Tetramethylpentane							
Forziati *et al.* (1949)	**20**	**316–396**	**6.4–104**	**0.19**	**0.014**	**0.9989**	**0.18**
Smith (1941)	15	331–423	12–199				0.17
2,3,3,4-Tetramethylpentane							
Forziati *et al.* (1949)	**18**	**332–416**	**6.4–104**	**0.19**	**0.014**	**0.999 87**	**0.27**
3,3-Diethylpentane							
Forziati *et al.* (1949)	**19**	**336–420**	**6.4–104**	**0.19**	**0.014**	**0.999 87**	**0.064**
Osborn and Scott (1980)	12	273–338	0.2–7	0.5	0.015	0.999 85	0.52
***n*-Decane**							
Allemand *et al.* (1986)	11	298–348	0.18–3.2	1	1	>0.995	0.74
Beaudoin and Kohn (1967)	3	348–423	0.86–53	[b]	13	0.995	0.2
Carruth and Kobayashi (1973)	8	244–311	0.0017–0.21			0.9985	16
Chirico *et al.* (1989)	**33**	**268–490**	**0.017–270**	**0.59**	**0.002**	**0.999 98**	**0.11**
Dejoz *et al.* (1996)	**37**	**315–458**	**0.52–133**	**2**	**0.24**	**0.995**[c]	**0.47**
Gehrig and Lentz (1983)	21	274–615	0.025–2000			0.995	2.6
Gierycz *et al.* (1988)	3	373–447	9.6–101	0.0066	0.0026	0.9995	0.12
Gregorowicz *et al.* (1987)	15	363–393	6.3–20	0.11	0.048	0.9995	0.18
Krafft (1882a)	2	380–446	13–101				4.3
Lee *et al.* (1992)	6	409–584	34–1320	0.3	0.077	0.99	1.1
Linder (1931)	4	269–282	0.022–0.063				11
Morgan and Kobayashi (1994)	16	323–588	0.87–1395	0.58	0.042	0.9985	0.16
Reamer and Sage (1963)	8	278–511	0.028–446	[b]	0.32	0.9934	9.9
Viton *et al.* (1996)	33	244–467	0.0015–164	2	0.21	0.99	0.63
Willingham *et al.* (1945)	19	368–448	7.6–104	0.07	0.0072	>0.996	0.058
Willman and Teja (1985)	6	373–394	9.4–21	1.6	0.95	0.99	1.3
Woringer (1900)	33	273–433	0.083–105				49

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum T_{min} and maximum T_{max} temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties 100$\Delta p/p$ at T_{min}	Uncertainties 100$\Delta p/p$ at T_{max}	Purity (mole fraction)	AAD (%)
***n*-Undecane**							
Camin and Rossini (1955)	20	378–470	5.5–105			0.9997	0.26
Krafft (1882a)	6	347–468	1.5–101				6.8
Stadnicki (1962a)	4	449–469	60–101				0.76
Viton *et al.* (1996)	46	254–469	0.0011–100	2	0.21		0.83
***n*-Dodecane**							
Allemand *et al.* (1986)	19	298–390	0.017–4.3	1	1	>0.995	1.1
Beale and Docksey (1935)	21	300–658	0.02–1770	[b]	0.14		4.7
Dejoz *et al.* (1996)	**38**	**344–502**	**0.44–134**	**2.3**	**0.22**	**0.997**[c]	**0.26**
Gierycz *et al.* (1985)	13	378–418	2.6–13	0.039	0.0084	0.9999	1
Keistler and Van Winkle (1952)	8	363–486	1.3–101				4.7
Krafft (1882a)	6	364–488	1.5–101				6.3
Morgan and Kobayashi (1994)	**13**	**353–588**	**0.73–671**	**0.67**	**0.047**	**0.9994**	**0.14**
Sasse *et al.* (1988)	37	264–371	0.000 59–1.8	2	2	0.98	2.6
Viton *et al.* (1996)	35	264–468	0.000 64–58	2	0.21	0.996	0.7
Willingham *et al.* (1945)	20	400–491	6.4–104	0.084	0.007	>0.9994	0.049
***n*–Tridecane**							
Camin and Rossini (1955)	14	412–509	5.5–103			0.9992	0.15
Krafft (1882a)	6	380–507	1.5–101				5.8
Sunner and Svenson (1979)	3	308–348	0.013–0.23	7.7	0.44		4.9
Viton *et al.* (1996)	33	274–467	0.000 48–35	2	0.21		0.63
***n*-Tetradecane**							
Allemand *et al.* (1986)	6	343–395	0.072–1.3	1	1	>0.995	0.81
Camin and Rossini (1955)	11	428–527	5.5–103			0.9993	0.19
Kneisl and Zondlo (1987)	24	405–525	2.1–98	4.8	0.15	0.998	0.52
Krafft (1882a)	6	396–526	1.5–101				4.5
Morgan and Kobayashi (1994)	16	373–588	0.44–343	1.1	0.052	0.9995	0.23
Sunner and Svenson (1979)	3	313–358	0.007–0.18	14	0.56		5.2
Viton *et al.* (1996)	34	284–467	0.000 41–21	2	0.21		0.97
Ward and Van Winkle (1954)	10	435–518	6.5–85			>0.987	4.8
***n*-Pentadecane**							
Allemand *et al.* (1986)	6	333–409	0.016–1.3	1	1	>0.995	3.6
Camin and Rossini (1955)	10	443–544	5.5–101			0.9993	0.1
Krafft (1882a)	6	410–544	1.5–101				3.3
Sunner and Svenson (1979)	3	333–373	0.012–0.2	8.3	0.5		24
Viton *et al.* (1996)	20	294–467	0.000 36–13	2	0.21	0.98	1.7
***n*-Hexadecane**							
Camin *et al.* (1954)	16	463–560	6.9–101			0.9996	0.17
Eggertsen *et al.* (1969)	10	299–413	0.000 21–0.82				3.3
Francis and Wood (1926)	4	410–435	0.71–2.6				6.8
Grenier-Loustalot *et al.* (1981)	4	358–418	0.036–1.2	3.8	0.44		4.8
Krafft (1882a)	6	424–561	1.5–101				3
Lee *et al.* (1992)	5	504–589	26–188	0.39	0.53	0.99	1.9
Mills and Fenton (1987)	11	389–560	0.25–102	2	0.022		0.58
Morgan and Kobayashi (1994)	**20**	**393–583**	**0.32–164**	**1.5**	**0.059**	**0.9994**	**0.51**
Myers and Fenske (1955)	26	354–559	0.027–101	5.2	0.43	>0.98	3
Parks and Moore (1949)	10	298–323	0.000 19–0.0031	1.5	1.2		10
Viton *et al.* (1996)	24	303–467	0.000 28–8	2	0.21		2.8
***n*-Heptadecane**							
Grenier-Loustalot *et al.* (1981)	5	358–434	0.015–1.4	9.1	0.43		5.7
Krafft (1882a)	6	437–576	1.5–101				2.6
Viton *et al.* (1996)	24	314–467	0.0003–5	2	0.21		1.5
***n*-Octadecane**							
Allemand *et al.* (1986)	11	335–440	0.0012–1	1	1	>0.995	2.9
Grenier-Loustalot *et al.* (1981)	5	358–434	0.0067–0.75	20	0.5		4.4
Krafft (1882a)	6	448–590	1.5–101				4
Macknick and Prausnitz (1979)	10	318–361	0.000 22–0.0097	2.3	2.2	>0.99	2.8
Morgan and Kobayashi (1994)	17	413–588	0.27–98	1.8	0.063	0.998	0.94
Myers and Fenske (1955)	23	376–568	0.027–67	5.2	0.44	>0.98	4
Viton *et al.* (1996)	16	333–467	0.000 83–3	2	0.21	0.97	2.1
***n*-Nonadecane**							
Grenier-Loustalot *et al.* (1981)	4	379–434	0.016–0.42	8.4	0.61		3.6

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum $T_{\min}$ and maximum $T_{\max}$ temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties $100\Delta p/p$ at $T_{\min}$	 $100\Delta p/p$ at $T_{\max}$	Purity (mole fraction)	AAD (%)
Krafft (1882a)	6	459–603	1.5–101				5
Morecroft (1964)	3	306–328	0.0000 19–0.000 21				7.6
Morgan and Kobayashi (1994)	16	423–588	0.26–74	1.9	0.066	0.992	1.3
Viton *et al.* (1996)	15	334–467	0.000 38–1.9	2	0.22		2.1
***n*-Eicosane**							
Chirico *et al.* (1989)	**29**	**388–626**	**0.016–121**	**0.64**	**0.002**	**0.9995**	**0.59**
Grenier-Loustalot *et al.* (1981)	5	358–434	0.0012–0.24	[b]	0.77		8.7
Macknick and Prausnitz (1979)	7	344–380	0.000 41–0.0091	2.3	2.2	>0.99	4.8
Morgan and Kobayashi (1994)	32	433–588	0.24–54	2	0.07	0.999	0.42
Myers and Fenske (1955)	21	395–573	0.027–40	5.2	0.5	>0.98	4.3
Piacente *et al.* (1991)	122	315–472	0.000 029–1.2			>0.99	24
Piacente *et al.* (1994)	28	347–388	0.000 32–0.019			0.99	26
Sasse *et al.* (1988)	21	363–467	0.0023–1.3	2	2	0.98	2.4
Schiessler and Whitmore (1955)	5	410–470	0.067–1.3			>0.95	1.4
Viton *et al.* (1996)	14	342–467	0.0004–1.2	2	0.22		1.9
***n*-Heneicosane**							
Grenier-Loustalot *et al.* (1981)	4	379–434	0.004–0.14	33	1.1		3.9
Mazee (1948)	8	440–468	0.21–0.83				3.5
Piacente *et al.* (1991)	86	326–477	0.000 049–1.1			>0.99	29
Piacente *et al.* (1994)	22	365–400	0.000 96–0.023			0.99	14
***n*-Docosane**							
Francis and Wood (1926)	9	462–509	0.27–3.6				21
Grenier-Loustalot *et al.* (1981)	4	379–434	0.0021–0.084	63	1.7		3.3
Morgan and Kobayashi (1994)	12	453–573	0.24–21	2	0.084	0.993	0.3
Piacente *et al.* (1991)	115	341–489	0.000 074–0.89			>0.99	28
Piacente *et al.* (1994)	23	372–410	0.000 64–0.029			0.99	25
Sasse *et al.* (1988)	16	353–462	0.0002–0.4	2	2	0.95	3.4
Young (1928)	3	494–519	1.5–4	0.92	0.35		5.1
***n*-Tricosane**							
Mazee (1948)	7	471–492	0.37–0.96				2.1
Piacente *et al.* (1991)	83	348–489	0.000 085–0.81			>0.99	17
Piacente *et al.* (1994)	40	370–416	0.000 32–0.022			0.99	20
***n*-Tetracosane**							
Francis and Wood (1926)	9	468–529	0.2–37				27
Grenier-Loustalot *et al.* (1981)	4	379–434	0.000 53–0.028	[b]	4.8		26
Mazee (1948)	6	473–499	0.27–0.87				2.3
Meyer and Stec (1971)	6	499–565	0.83–9				1.9
Morgan and Kobayashi (1994)	**13**	**453–588**	**0.09–17**	**5.3**	**0.087**	**0.995**	**0.91**
Piacente and Scardala (1990)	31	451–496	0.062–0.62	[b]	23	0.995	47
Piacente *et al.* (1991)	78	343–523	0.000 01–1.3			>0.99	28
Piacente *et al.* (1994)	40	386–429	0.000 72–0.025			0.99	17
Sasse *et al.* (1988)	12	373–462	0.000 25–0.15	2	2	0.97	6.2
Young (1928)	3	513–539	1.5–4	0.92	0.35		4.4
***n*-Pentacosane**							
Grenier-Loustalot *et al.* (1981)	4	379–434	0.000 27–0.017	[b]	7.7		3.2
Piacente and Scardala (1990)	19	461–498	0.078–0.5	[b]	28	0.995	23
Piacente *et al.* (1991)	83	356–531	0.000 033–1.3			>0.99	22
Piacente *et al.* (1994)	36	306–434	0.0013–0.029			0.99	21
***n*-Hexacosane**							
Francis and Wood (1926)	5	497–542	0.28–3.5				22
Grenier-Loustalot *et al.* (1981)	4	379–434	0.000 13–0.011	[b]	13		1.5

TABLE 4. Summary of experimental hydrocarbon vapor pressure data, including total uncertainty in p^{1+g} at the minimum T_{min} and maximum T_{max} temperature of the measurements—Continued

Author[a]	No. of points	Temp. range K	Pressure range (kPa)	Uncertainties		Purity (mole fraction)	AAD (%)
				$100\Delta p/p$ at T_{min}	$100\Delta p/p$ at T_{max}		
Piacente and Scardala (1990)	35	455–519	0.037–0.81	[b]	18	0.995	12
Piacente *et al.* (1991)	109	356–546	0.000 02–1.6			>0.99	34
Piacente *et al.* (1994)	39	391–437	0.000 32–0.019			0.99	20
Young (1928)	3	532–556	1.5–4	0.92	0.34		7.8
***n*-Heptacosane**							
Morecroft (1964)	6	351–435	0.000 003 7–0.0067				17
Piacente *et al.* (1991)	5	377–390	0.000 089–0.000 33			>0.99	39
Piacente *et al.* (1994)	21	408–440	0.000 49–0.0093			0.99	32
***n*-Octacosane**							
Chirico *et al.* (1989)	**13**	**453–575**	**0.013–3.9**	**0.76**	**0.0043**	**0.999 84**	**2.8**
Francis and Wood (1926)	9	507–561	0.29–3.7				20
Grenier-Loustalot *et al.* (1981)	3	398–434	0.000 13–0.0035	[b]	38		23
Mazee (1948)	8	494–522	0.15–0.53				4.2
Morgan and Kobayashi (1994)	14	483–588	0.082–6	5.8	0.12	0.993	0.81
Piacente and Scardala (1990)	19	473–515	0.039–0.38	[b]	37	0.995	9.3
Piacente *et al.* (1991)	67	356–568	0.000 013–2.1			>0.99	23
Piacente *et al.* (1994)	36	407–456	0.000 4–0.023			0.99	19
Young (1928)	3	548–575	1.5–4	0.92	0.35		6.4
***n*-Nonacosane**							
Francis and Wood (1926)	5	521–564	0.33–2.5				16
Piacente *et al.* (1991)	5	377–410	0.000 018–0.000 79			>0.99	45
Young (1928)	2	559–568	1.5–2	0.92	0.68		18
***n*-Triacontane**							
Francis and Wood (1926)	5	515–585	0.23–4.1				19
Mazee (1948)	7	524–548	0.28–0.78				5.6
Piacente *et al.* (1994)	42	422–487	0.000 48–0.08			0.99	20
Young (1928)	3	566–597	1.5–4	0.92	0.35		22
***n*-Hentriacontane**							
Mazee (1948)	7	517–553	0.15–0.72				7.0
Piacente *et al.* (1994)	29	433–474	0.000 64–0.021			0.99	20
***n*-Dotriacontane**							
Piacente *et al.* (1994)	35	437–477	0.000 8–0.021			0.99	28
***n*-Tritriacontane**							
Piacente *et al.* (1994)	21	435–482	0.000 32–0.018			0.99	19
***n*-Tetratriacontane**							
Francis and Wood (1926)	5	558–611	0.32–4				22
Mazee (1948)	7	537–559	0.16–0.42				2.0
Piacente *et al.* (1994)	27	446–497	0.000 48–0.031			0.99	19
Young (1928)	3	598–625	1.5–4	0.92	0.35		31
***n*-Pentatriacontane**							
Mazee (1948)	7	553–570	0.23–0.49				3.1
***n*-Hexatriacontane**							
Mazee (1948)	7	550–572	0.16–0.40				2.6
Piacente *et al.* (1994)	35	452–516	0.000 32–0.052			0.99	26
***n*-Heptatriacontane**							
Piacente *et al.* (1994)	40	471–511	0.000 96–0.022			0.99	21
***n*-Octatriacontane**							
Piacente *et al.* (1994)	38	471–511	0.000 64–0.017			0.99	21
***n*-Tritetracontane**							
Mazee (1948)	8	581–612	0.13–0.52				17

[a] Rows summarizing the measurements used in the regression analysis have been bolded.

[b] Uncertainty greater than the experimental pressure.

[c] Weight fraction purity.

TABLE 5. Coefficients of the generalized vapor pressure equation, Eq. (12), determined in this work

k	N_k
1	−5.968 127 116 539
2	1.244 160 804 719
3	−0.501 340 221 969
4	−1.316 444 840 726
5	−4.589 426 828 138
6	1.365 162 911 745
7	−5.162 331 161 063
8	−5.678 478 208 052
9	−2.798 018 429 501
10	3.010 247 883 995
11	−7.634 352 378 867
12	−0.178 136 926 230

4.2. Isomers of the *n*-Alkanes

Equation (12), for which the coefficients were adjusted based solely on vapor pressure data for the normal alkanes, may also be used to determine the vapor pressures of branched alkanes. To do so requires the branched alkane critical temperature, critical pressure, and ω. These properties can be obtained from knowledge of one of the following two options: (1) direct measurement of the critical state and boiling temperature at ambient pressure; or (2) measurements of the vapor pressure at temperatures over about half the fluid range combined with Eq. (12) and a regression algorithm. The second option was verified for n-heptane since data are available over nearly the whole fluid range. In this case, the data of Willingham *et al.* (1945) from 299 to 372 K were used in a nonlinear regression to determine both critical parameters and the value of ω. The resulting values were $T_c = 537.939\,\mathrm{K}$, $p_c = 2.6459\,\mathrm{MPa}$, and $\omega = 0.341\,07$. These results are in reasonable agreement with those listed in Table 2 ($T_c = 540.13\,\mathrm{K}$, $p_c = 2.727\,\mathrm{MPa}$, and $\omega = 0.336\,02$). The data reported by Weber (1999) over the temperature range from 335 to 503 K were compared with Eq. (12) using the parameters obtained from option (2) and listed above. The average absolute deviations of the Weber (1999) data was $0.0006 \cdot p^{1+g}$, which is insignificantly different from $0.0007 \cdot p^{1+g}$ obtained with the parameters listed in Table 2, even though the upper temperature of the Weber data is both 131 K above the highest cited temperature of Willingham *et al.* and 37 K from the critical point. In other similar comparisons, the T_c obtained from option (2) was found to differ from experimental values of the critical temperature, however, the vapor pressures predicted by a self consistent set of parameters obtained from option (2) provided an accurate representation of the vapor pressure data.

Although Eq. (12) can be applied to all isomers of the n-alkanes, Table 6 reports values of the critical parameters and of ω only for the isomers of n-butane through n-octane, and for several of the isomers of n-nonane. If the critical temperature, critical pressure, and normal boiling point (or other saturation point) of an isomer are known, the value of ω can be estimated using

$$\omega = \frac{-\mathrm{Pr}^{(1)} - \sqrt{(\mathrm{Pr}^{(1)})^2 - 4[\mathrm{Pr}^{(0)} - T_r \ln(p^{1+g}/p_c)]\mathrm{Pr}^{(2)}}}{2\mathrm{Pr}^{(2)}}, \tag{25}$$

where $\mathrm{Pr}^{(0)}$, $\mathrm{Pr}^{(1)}$, and $\mathrm{Pr}^{(2)}$ are obtained from Eqs. (13), (14), and (15) at the temperature of the saturation point. As an example, the value of ω calculated from Eq. (25) is 0.276 67 for the data point at 314.70 K and 0.053 654 MPa for 2-methylpentane from Willingham *et al.* (1945). The critical parameters used in this example are those from Table 6. The calculated value of ω is very similar to the value given in Table 6, $\omega = 0.276\,52$, which was fit to multiple data points.

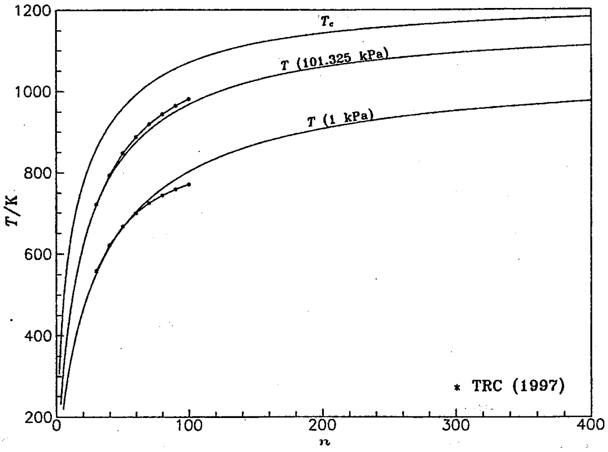

FIG. 3. The variation in critical temperature T_c, normal boiling temperature $T(p = 101.325\,\mathrm{kPa})$ and boiling temperature at a pressure of 1 kPa $T(p = 1\,\mathrm{kPa})$ obtained from Eq. (12) as a function of the number of carbon atoms n for C_nH_{2n+2} with $n \leq 400$.

The critical temperatures and pressures used for the branched alkanes were mostly obtained from the literature and are listed in Table 6. Data used in determining the values of ω for each isomer are indicated in Table 4. For several of the isomers, systematic errors occurred when optimizing the parameter ω. This generally indicated that either the critical temperature or critical pressure (or both) was in error and, given sufficient data, the critical pressure was determined during the fitting process at the same time as ω. This procedure was adopted for 2-methylbutane, 3,3-dimethylpentane, 2-methylheptane, 2,2,4-trimethylpentane, 2,2,5-trimethylhexane, and 3,3-diethylpentane.

5. Comparisons

The experimental vapor pressure measurements used in the regression analysis are shown as deviations from Eq. (12) in Figs. 4–22. For clarity, data were selected for inclusion in the plots on the basis of two criteria. First, data sets containing one to five data points were omitted when there was a large number of data sources for that fluid and, second, data

TABLE 6. Values of T_c, p_c, and ω for the branched alkanes used in Eq. (12)

Substance	Reference	T_c/K	p_c/MPa	ω	T_b/K[b]
2-Methylpropane	Daubert (1996)	407.8	3.640	0.190 29	261.403
2-Methylbutane	Ewing and Goodwin (1991)	460.9	3.386[a]	0.226 59	300.992
2,2-Dimethylpropane	Daubert (1996)	433.8	3.196	0.202 18	282.722
2-Methylpentane	Daubert (1996)	497.7	3.04	0.276 52	333.342
3-Methylpentane	Daubert (1996)	504.6	3.12	0.268 79	336.377
2,2-Dimethylbutane	Daubert (1996)	489.0	3.10	0.234 53	322.860
2,3-Dimethylbutane	Daubert (1996)	500.0	3.15	0.249 18	331.075
2-Methylhexane	Daubert (1996)	530.4	2.74	0.319 96	363.107
3-Methylhexane	Daubert (1996)	535.2	2.81	0.313 71	364.914
2,2-Dimethylpentane	Daubert (1996)	520.5	2.77	0.283 21	352.363
2,3-Dimethylpentane	Daubert (1996)	537.3	2.91	0.291 03	362.850
2,4-Dimethylpentane	Daubert (1996)	519.8	2.74	0.297 35	353.648
3,3-Dimethylpentane	Daubert (1996)	536.4	2.93[a]	0.263 76	359.185
2,2,3-Trimethylbutane	Daubert (1996)	531.1	2.95	0.250 44	354.019
3-Ethylpentane	Daubert (1996)	540.6	2.89	0.303 86	366.634
2-Methylheptane	Daubert (1996)	559.7	2.49[a]	0.360 52	390.704
3-Methylheptane	Daubert (1996)	563.6	2.55	0.354 92	392.008
4-Methylheptane	Daubert (1996)	561.7	2.54	0.354 90	390.824
2,2-Dimethylhexane	Daubert (1996)	549.8	2.53	0.328 05	380.007
2,3-Dimethylhexane	Daubert (1996)	563.5	2.63	0.333 69	388.661
2,4-Dimethylhexane	Daubert (1996)	553.5	2.56	0.332 09	382.554
2,5-Dimethylhexane	Daubert (1996)	550.0	2.49	0.342 81	382.183
3,3-Dimethylhexane	Daubert (1996)	562.0	2.65	0.311 52	385.054
3,4-Dimethylhexane	Daubert (1996)	568.8	2.69	0.327 09	390.811
2,2,3-Trimethylpentane	Daubert (1996)	563.5	2.73	0.292 46	382.990
2,2,4-Trimethylpentane	Daubert (1996)	543.8	2.56[a]	0.297 01	372.323
2,3,3-Trimethylpentane	Daubert (1996)	573.5	2.82	0.284 79	387.759
2,3,4-Trimethylpentane	Daubert (1996)	566.4	2.73	0.307 00	386.513
2,2,3,3-Tetramethylbutane	Reid *et al.* (1987)	567.8	2.87	0.250 00	379.438
3-Ethylhexane	Daubert (1996)	565.5	2.61	0.346 45	391.630
2-Methyl-3-ethylpentane	Daubert (1996)	567.1	2.70	0.319 86	388.750
3-Methyl-3-ethylpentane	Daubert (1996)	576.5	2.81	0.296 73	391.228
2,2,3-Trimethylhexane	Reid *et al.* (1987)	588.0	2.49	0.331 01	407.330
2,2,4-Trimethylhexane	Matteson (1950)	575.4	2.30	0.323 86	400.828
2,2,5-Trimethylhexane	Daubert (1996)	569.8	2.43[a]	0.346 22	397.185
2,4,4-Trimethylhexane	Matteson (1950)	579.9	2.38	0.333 85	403.713
2,2,3,3-Tetramethylpentane	Daubert (1996)	607.5	2.74	0.297 44	413.325
2,2,3,4-Tetramethylpentane	Daubert (1996)	592.6	2.60	0.305 84	406.118
2,2,4,4-Tetramethylpentane	Daubert (1996)	574.6	2.49	0.305 17	395.320
2,3,3,4-Tetramethylpentane	Daubert (1996)	607.5	2.72	0.305 51	414.532
3,3-Diethylpentane	Reid *et al.* (1987)	610.0	2.58[a]	0.314 36	419.311

[a] Values of the critical pressures for 2-methylbutane, 3,3-dimethylpentane, 2-methylheptane, 2,2,4-trimethylpentane, 2,2,5-trimethylhexane, and 3,3-diethylpentane were obtained by regression analysis described in Sec. 4.2.

[b] Calculated from Eq. (12) at 0.101 325 MPa

sets for which most of the deviations exceed the scale of the plot are not shown. For each of the normal alkanes up to n-heptane, at least 25 separate articles report measurement for each alkane, some with significantly high deviations from Eq. (12). In order to show clearly the agreement between Eq. (12) and the measurements of highest precision, two plots with differing ordinates axes were used for each fluid. For methane through n-butane, the top graph shows deviations less than $0.005 \cdot p^{1+g}$, while the lower graph shows deviations less than $0.04 \cdot p^{1+g}$. For those deviations that exceed the ordinate scale, the symbols are shown at the top or bottom of the plot.

Many wide range vapor pressure equations have been published for various pure alkanes over the range from the triple point to the critical point. These equations are based either on extensive measurements over a wide temperature range or

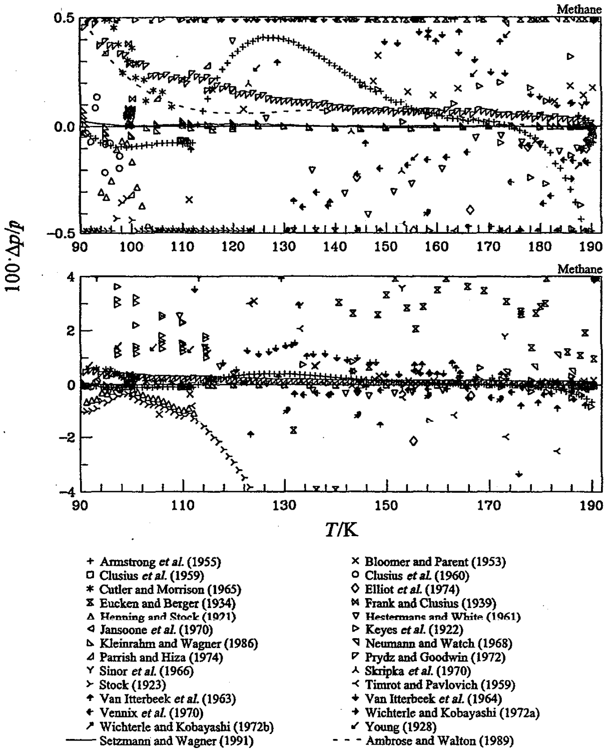

FIG. 4. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for methane.

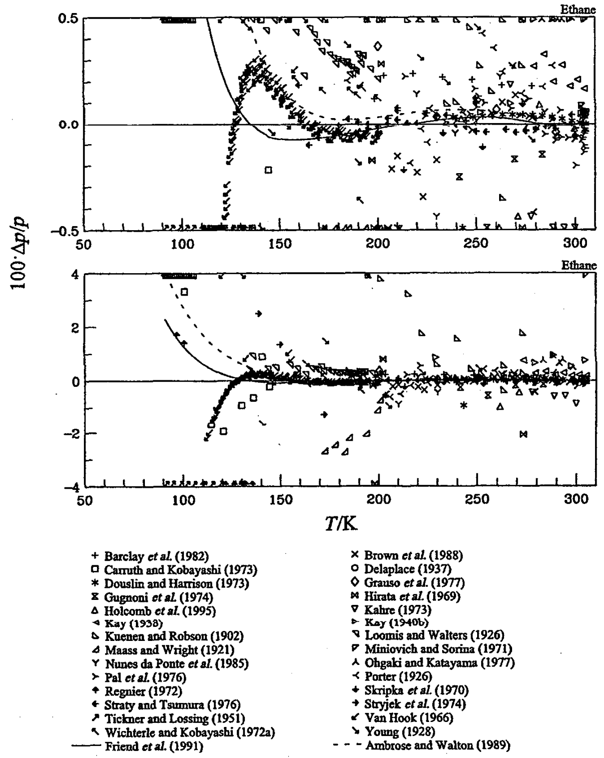

FIG. 5. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for ethane.

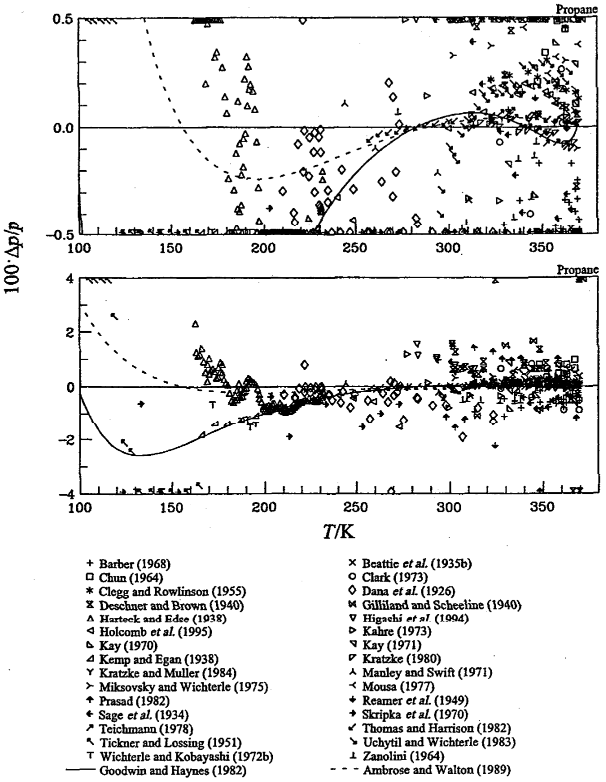

FIG. 6. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for propane.

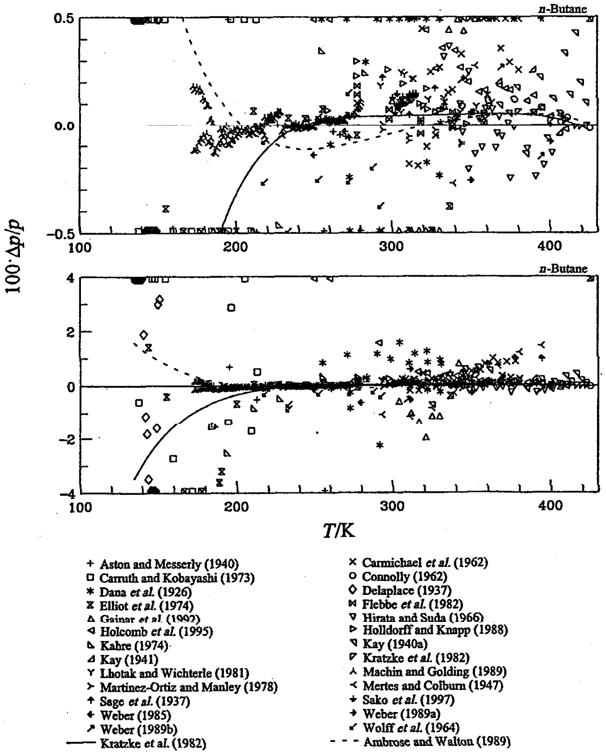

FIG. 7. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for *n*-butane.

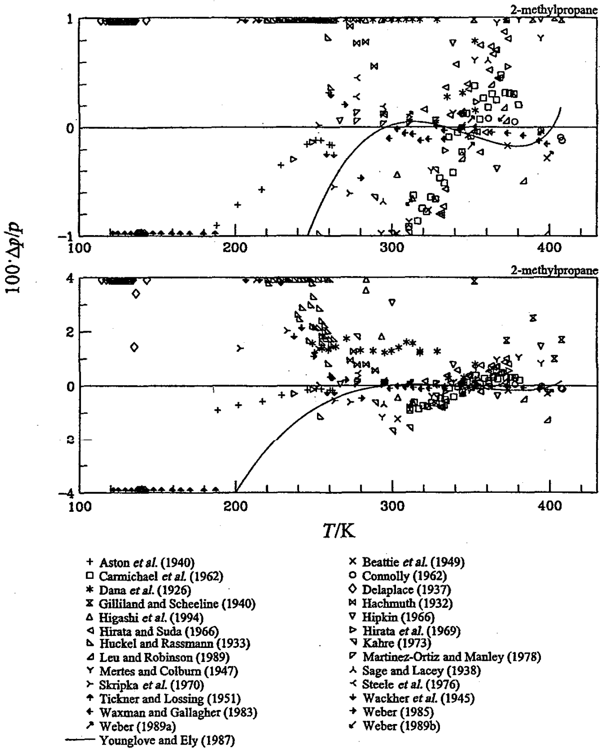

FIG. 8. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for 2-methylpropane.

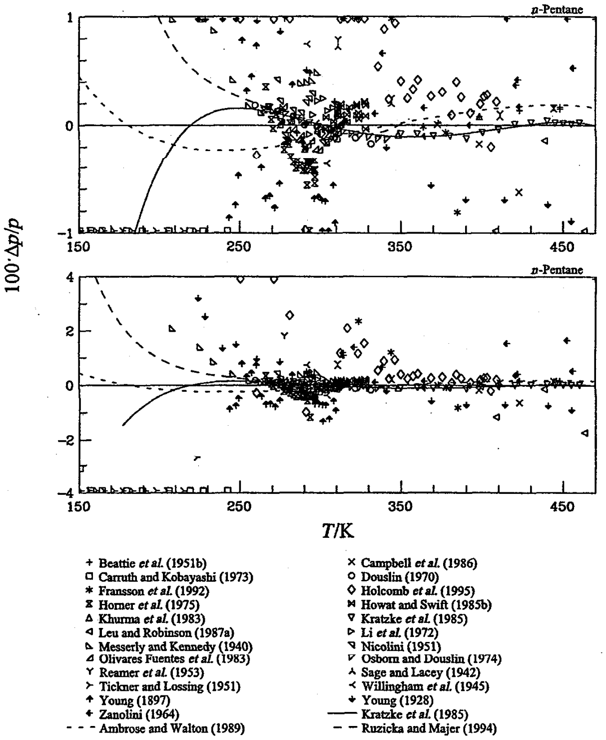

FIG. 9. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for n-pentane.

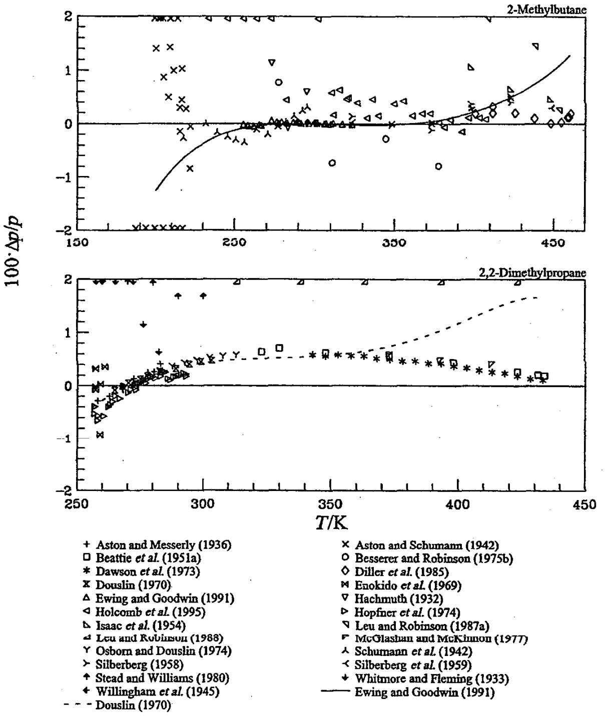

FIG. 10. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for 2-methylbutane (top) and 2,2-dimethylpropane (bottom).

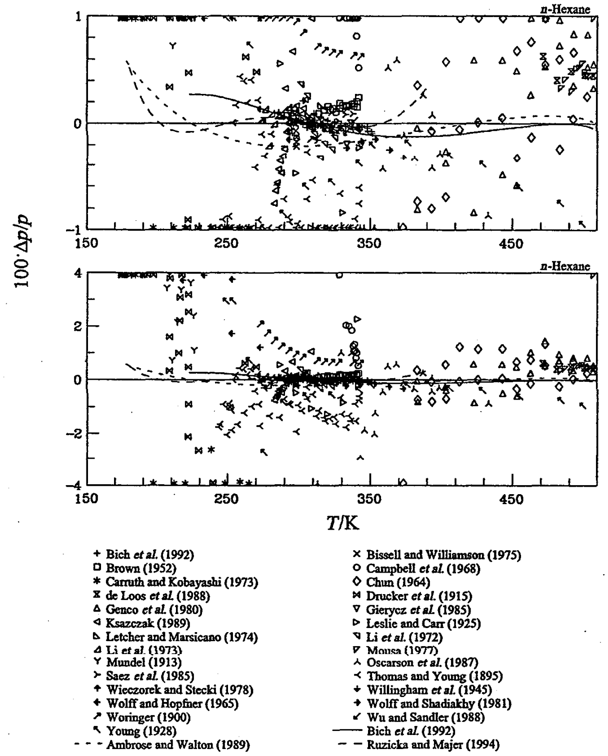

FIG. 11. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for n-hexane.

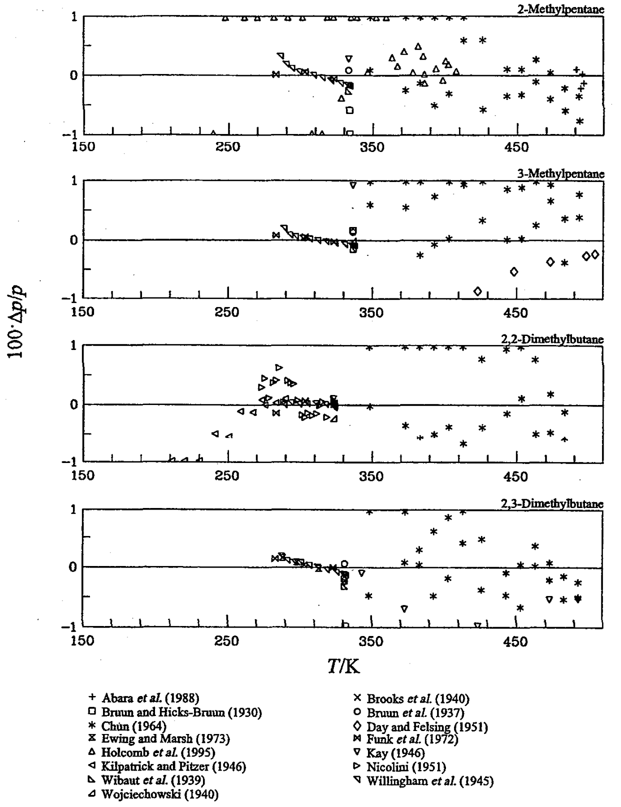

FIG. 12. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) 2-methylpentane, (2) 3-methylpentane, (3) 2,2-dimethylbutane, and (4) 2,3dimethylbutane.

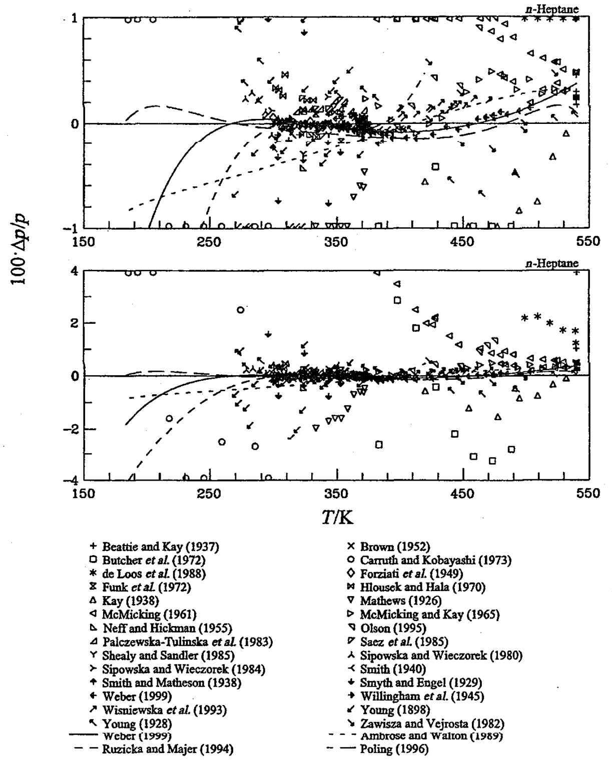

FIG. 13. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for n-heptane.

a comprehensive review of existing literature data. Vapor pressure equations are shown as solid lines in Figs. 4–13 for the following fluids: methane (Setzmann and Wagner, 1991), ethane (Friend *et al.*, 1991), propane (Goodwin and Haynes, 1982), n-butane (Kratzke *et al.*, 1982), 2-methylpropane (Younglove and Ely, 1987), n-pentane (Kratzke *et al.*, 1985), 2-methylbutane (Ewing and Goodwin, 1991), 2,2-dimethylpropane (Douslin, 1970), n-hexane (Bich *et al.*, 1992), and n-heptane (Weber, 1999).

Additional vapor pressure equations that have been developed to represent the properties of groups of alkanes are shown in the figures for further comparison. Values calculated from the n-alkane vapor pressure correlation of Ambrose and Walton (1989) are shown for n-alkanes up to n-eicosane, and values calculated from the correlation of Morgan and Kobayashi (1992) are shown for n-eicosane and higher. Ruzicka and Majer (1994), (1996) developed equations for the vapor pressures of alkanes at low temperatures between the triple point and the boiling point by extrapolating the vapor pressure using the enthalpy of vaporization and the heat capacities of the liquid and ideal gas. Values calculated from their equations are shown for the n-alkanes from n-pentane to n-eicosane and for several of the isomers of octane. For n-heptane, calculated values from the equations of Poling (1996) and Weber (1999) are shown. Poling used the Clapeyron equation to calculate vapor pressures at low temperatures from heat capacity measurements. Weber used heat capacities of the saturated liquid and ideal gas along with virial coefficients to calculate thermodynamic values of the vapor pressure at temperatures below 300 K.

For $C_{21}H_{44}$ through $C_{43}H_{88}$, the data of Mazee (1948) were tabulated at $p^{1+g}=400\,\mathrm{Pa}$ and shown graphically at pressures between 134 and 959 Pa in the original work. The values listed in Table 7 are estimates obtained from the plot given by Mazee. The first listed temperature for each alkane refers to the pressure at 400 Pa. The extrapolation behavior of Eq. (12) for alkanes greater than n-octacosane (the largest alkane for which experimental data were fit) was monitored during the fitting process, and the final equation represents the data of Mazee (1948) for n-hexatriacontane ($C_{36}H_{74}$) with an average deviation of $0.026\cdot p^{1+g}$.

The data selected for determining the coefficients given in Table 5 were described in the previous section. Clearly, the excellent agreement between vapor pressures obtained from Eq. (12) and from experimental measurements both verify the approach taken in this work and the generalization of the vapor pressure equation. Comparisons to experimental and predicted values for n-heptane and other fluids demonstrate that our approach should extrapolate well to low temperatures. In addition, data fitted from fluids at low temperatures will influence the vapor pressure representation of other fluids without similar data.

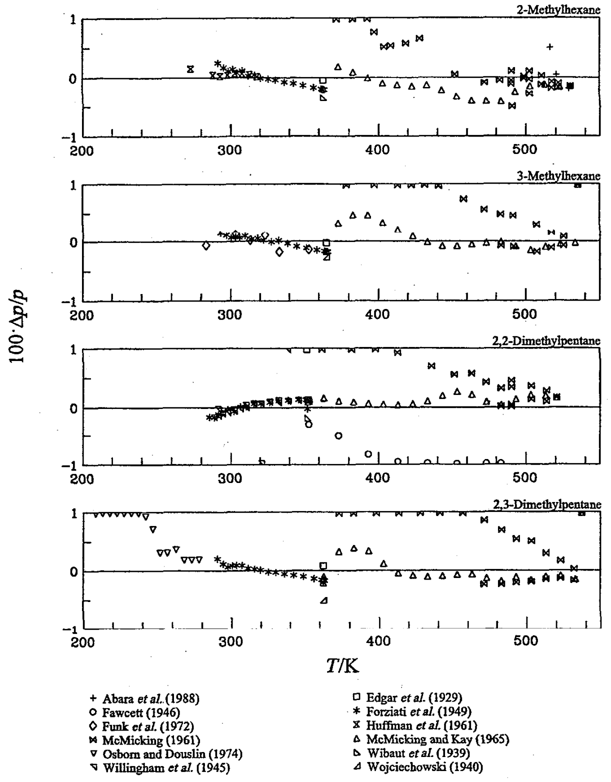

FIG. 14. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) 2-methylhexane, (2) 3-methylhexane, (3) 2,2-dimethylpentane, and (4) 2,3-dimethylpentane.

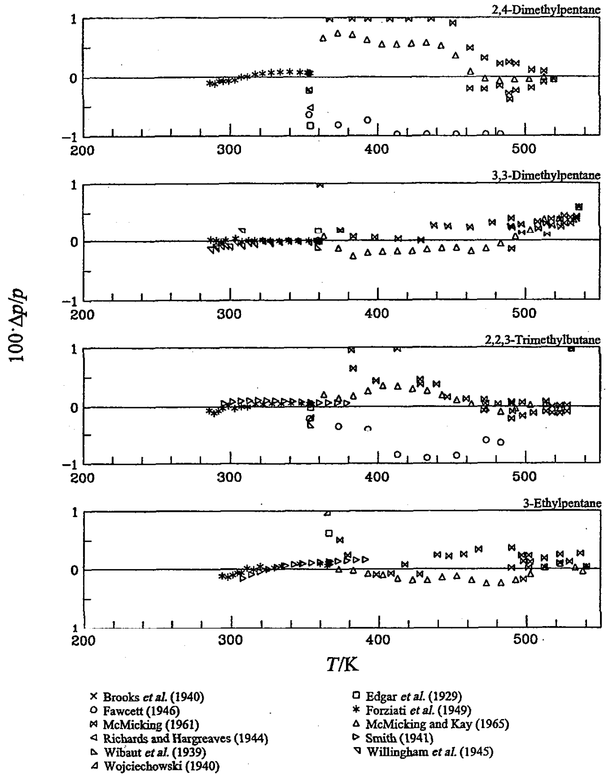

FIG. 15. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) 2,4-dimethylpentane, (2) 3,3-dimethylpentane, (3) 2,2,3-trimethylbutane, and (4) 3-ethylpentane.

6. Uncertainty of the Model

The average absolute deviations (AADs) between vapor pressures obtained from Eq. (12) and experimental values are listed in Table 4. The percent deviation in vapor pressure is defined as

$$\%\Delta p/p = 100[(p_{\text{exp}}^{1+g} - p_{\text{calc}}^{1+g})/p_{\text{exp}}^{1+g}]. \qquad (26)$$

At pressures greater than 1 kPa, the uncertainty of the vapor pressure equation presented here is as follows: $0.0001 \cdot p^{1+g}$ for methane, $0.001 \cdot p^{1+g}$ for ethane, propane, and n-butane, $0.002 \cdot p^{1+g}$ for n-pentane through n-octane, 2-methylpropane, and 2-methylbutane, $0.005 \cdot p^{1+g}$ for 2,2-dimethylpropane, n-nonane, n-decane, and the isomers of hexane through nonane, $0.01 \cdot p^{1+g}$ for n-undecane to n-hexadecane, $0.02 \cdot p^{1+g}$ for n-heptadecane to n-eicosane, $0.05 \cdot p^{1+g}$ for n-heneicosane to n-octacosane, and 0.10 $\cdot p^{1+g}$ for n-nonacosane to n-hexatriacontane. The uncertainty in the correlation is determined at the 99.5% confidence interval by two times the AAD for each substance. For fluids with limited experimental data sets, the uncertainties so determined must be considered predictions, until additional experimental values are available to verify the behavior of Eq. (12). However, we expect for engineering applications that vapor pressures obtained from Eq. (12) with

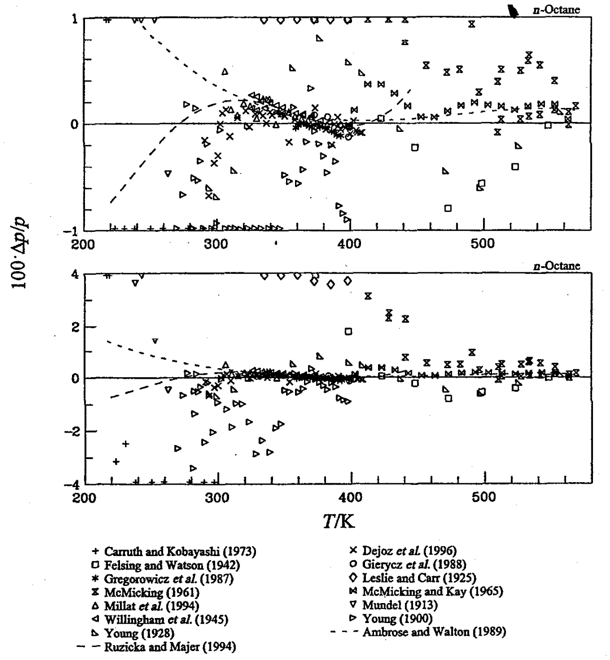

FIG. 16. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for n-octane.

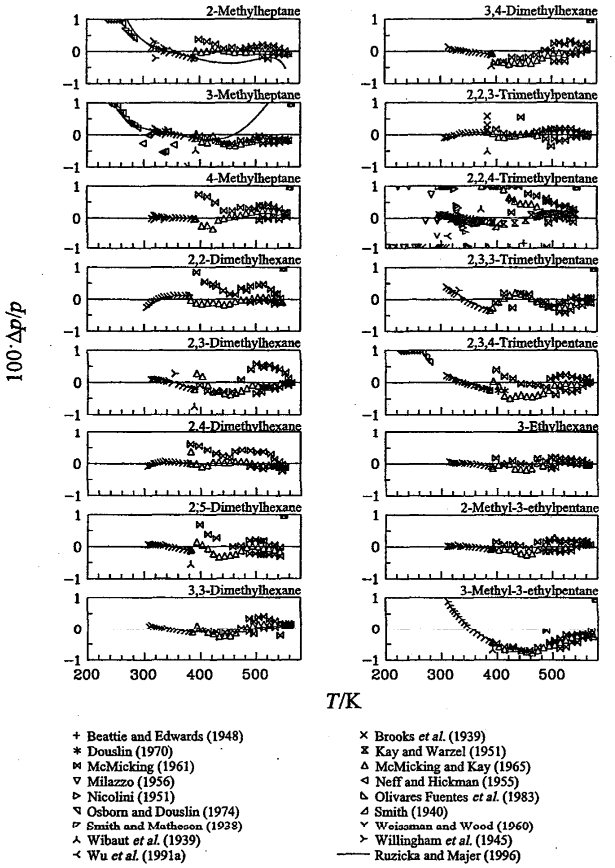

FIG. 17. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) 2-methylheptane, (2) 3-methylheptane, (3) 4-methylheptane, (4) 2,2-dimethylhexane, (5) 2,3-dimethylhexane, (6) 2,4-dimethylhexane, (7) 2,5-dimethylhexane, (8) 3,3-dimethylhexane, (9) 3,4-dimethylhexane, (10) 2,2,3-trimethylpentane, (11) 2,2,4-trimethylpentane, (12) 2,3,3-trimethylpentane, (13) 2,3,4-trimethylpentane, (14) 3-ethylhexane, (15) 2-methyl-3-ethylpentane, and (16) 3-methyl-3-ethylpentane.

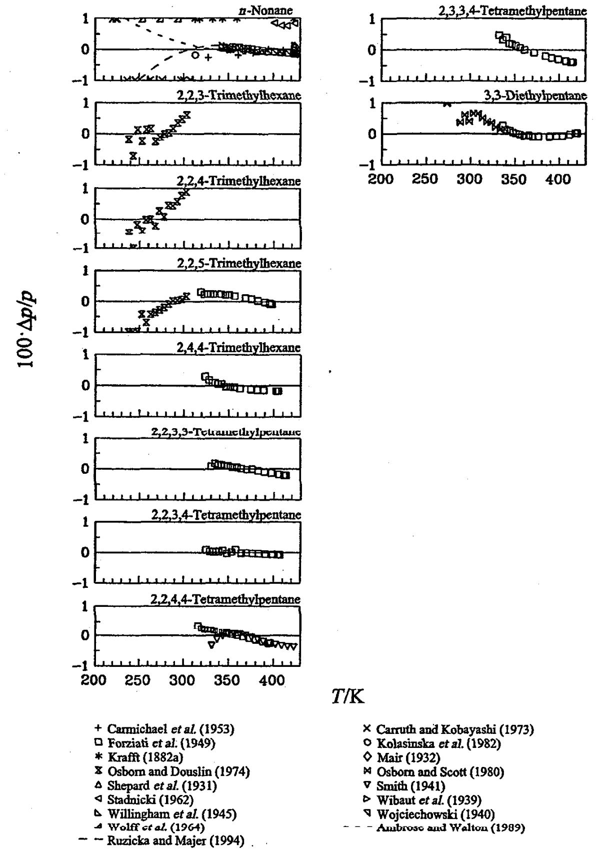

FIG. 18. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) n-nonane, (2) 2,2,3-trimethylhexane, (3) 2,2,4-trimethylhexane, (4) 2,2,5-trimethylhexane, (5) 2,4,4-trimethylhexane, (6) 2,2,3,3-tetramethylpentane, (7) 2,2,3,4-tetramethylpentane, (8) 2,2,4,4-tetramethylpentane, (9) 2,3,3,4-tetramethylpentane, and (10) 3,3-diethylpentane.

coefficients from Table 5 are sufficient. The basis for this statement of accuracy is given in this section.

Vapor pressures determined from this correlation lie within the experimental uncertainty for the most accurate data. We regard the data selected for use in determining the coefficients given in Table 5 (indicated in Table 4) as accurate and consistent with each other. Although data for the isomers were not used in the fit, the accuracy of the correlation for branched alkanes appears to be indistinguishable from that for the normal alkanes, substantiating the general applicability of the functional form used here.

Below the normal boiling point pressure, vapor pressures calculated with Eq. (12) deviate from the correlation of Ambrose and Walton (1989) for $n \leqslant 20$ by as much as 0.05 $\cdot p^{1+g}$. However, the vapor pressures are often in the range of 20 mPa–400 Pa, and percent differences are somewhat misleading because there may be only one to three significant figures in the reported data. The differences in pressure often approach the magnitude of the reported values at very low pressures. The differences between the Ambrose and Walton correlation and this work at these low pressures are well within the combined uncertainties of both correlations and well within the estimated uncertainties of the experimental data.

For methane, as illustrated in Fig. 4, the correlation developed in this work deviates on average by $0.000\,07 \cdot p^{1+g}$ from values calculated using the equation of Setzmann and Wagner (1991) which was based on the extensive accurate measurements reported by Kleinrahm and Wagner (1986). The generalized correlation of this work is consistent with that of Setzmann and Wagner within the experimental uncertainty of the data.

For ethane, the experimental vapor pressures reported by Van Hook (1966) were not fitted since the trends of the data near 170 K do not follow the trends of the data of Straty and Tsumura (1976), which we consider reliable. Other low temperature data were not included in the fit due to their large scatter. The same philosophy was followed for other fluids at low temperatures. Data that were judged to be questionable were not used in the fit. Rather, calculated vapor pressures

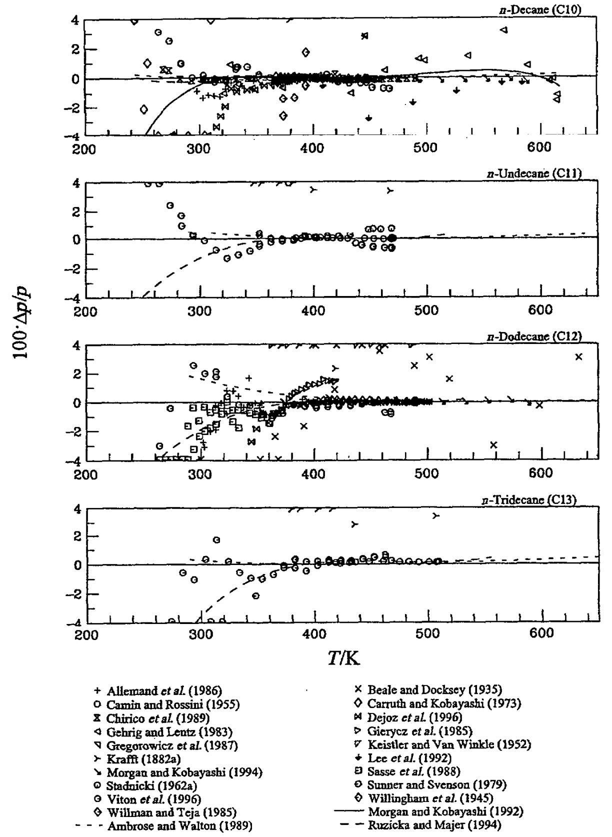

FIG. 19. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) n-decane, (2) n-undecane, (3) n-dodecane, and (4) n-tridecane.

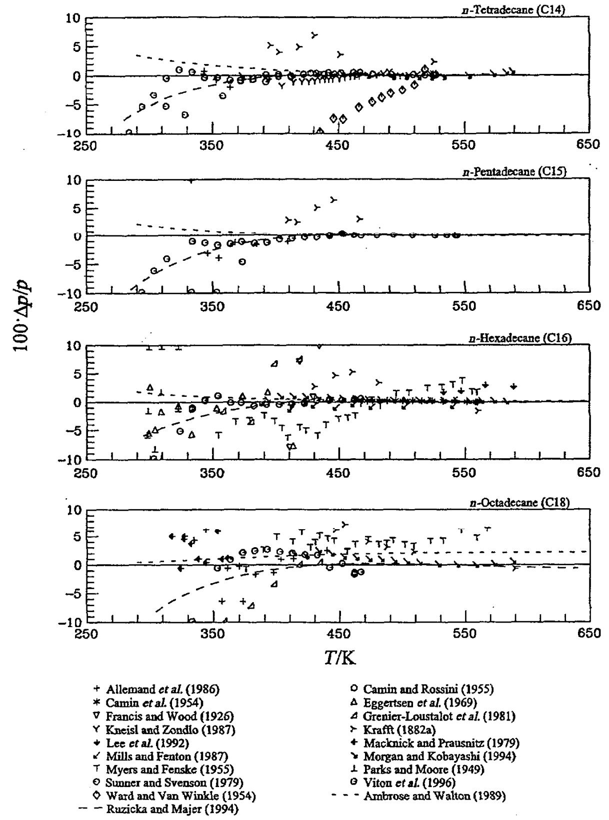

FIG. 20. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) n-tetradecane, (2) n-pentadecane, (3) n-hexadecane, and (4) n-octadecane.

for these fluids were influenced by the behavior of other fluids in the generalization. For example, much of the low temperature behavior of the equation for ethane and propane comes from fitting the data of Kleinrahm and Wagner (1986) for methane and Machin and Golding (1989) for n-butane. If inconsistent data for ethane or propane were used in the fit, errors in calculated values for methane and n-butane increased.

In general, values from the correlation deviate from the data for 2,2-dimethylpropane by as much as $0.005 \cdot p^{1+g}$. 2,2-Dimethylpropane is the only spherical molecule, other than methane, in the group of fluids studied. Figure 10 indicates a systematic deviation between measured and calculated values which cannot be explained. A separate equation was developed for 2,2-dimethylpropane that represents the experimental data within $0.001 \cdot p^{1+g}$, given by

$$\ln\left(\frac{p^{1+g}}{p_c}\right) = \frac{1}{T_r}(a\tau + b\tau^{1.5} + c\tau^{2.5} + d\tau^5), \qquad (27)$$

where $a = -6.9511$, $b = 1.5422$, $c = -1.7735$, $d = -3.3642$, $T_c = 433.8$ K, and $p_c = 3.1987$ MPa. Comparisons of experimental vapor pressure measurements with values calculated from this equation are shown in Fig. 23. The normal boiling point temperature calculated from this equation is 282.644 K.

The only available experimental data for 2,2,3,3-tetramethylbutane are six data points of Calingaert *et al.* (1944). These data are not shown in Fig. 17. They span the temperature range from 374 to 383 K, and the maximum deviation in vapor pressure is $0.002 \cdot p^{1+g}$. The behavior of the correlation for this fluid at temperatures outside this range cannot be verified without further experimental data.

For some isomers, Figs. 17 and 18 show systematic deviations between the reported data from various sources and the calculated values. The magnitudes of these deviations are generally less than $0.01 \cdot p^{1+g}$. Examples are 3-methyl-3-ethylpentane and 2,2,5-trimethylhexane. Some of the data of Osborn and Douslin (1974) for various fluids, e.g., 2,3-dimethylpentane, 2-methylheptane, 3-methylheptane, 2,3,4-trimethylpentane, and 2,2,5-trimethylhexane, appear to disagree systematically with values from this correlation. The uncertainties of these data were not given by the authors, so the consistency of these data with values calculated by the correlation given here is uncertain. However, the disagreement occurs at pressures less than 200 Pa. At such pressures, large relative differences are caused by numerically small

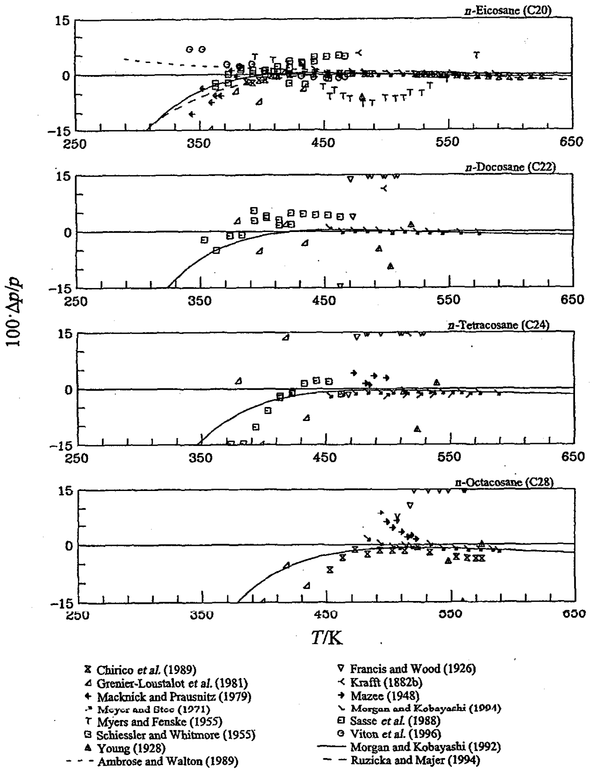

FIG. 21. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) n-eicosane, (2) n-docosane, (3) n-tetracosane, and (4) n-octacosane.

differences in low pressures as explained earlier.

One of the advantages of the correlation presented here can be seen when comparing the equation of Ambrose and Walton (1989) (for which the parameters T_c, p_c, and ω were not generalized as done in this work) with experimental data for n-heptadecane and n-nonadecane. In 1989, the data of Viton *et al.* (1996) and Morgan and Kobayashi (1994) were not available and were not used in the fit of Ambrose and Walton. Rather, the equation of Ambrose and Walton generally follows the data of Krafft (1882a). For the equation developed here, no data were used in the fit for these two fluids, but the equation represents the data of Viton *et al.* and Morgan and Kobayashi within their uncertainties as a result of generalizing T_c, p_c, and ω and of fitting other newer data at $n=16$, $n=20$, and $n=24$.

The values of Piacente and co-workers (1990), (1991), and (1994) are generally not consistent with values from other sources. For example, for n-eicosane, the average absolute deviation is about $0.25 \cdot p^{1+g}$ for the values by Piacente but is less than $0.02 \cdot p^{1+g}$ for the data of Chirico *et al.* (1989), Morgan and Kobayashi (1994), and Viton *et al.* (1996). These large deviations are typical for all the systems measured by Piacente. The deviations between the experimental data of Piacente and Eq. (12) are not shown in the figures.

The graphical data of Mazee (1948) for $C_{43}H_{88}$ disagree with values calculated using Eq. (12) by as much as $0.2 \cdot p^{1+g}$. Since Eq. (12) extrapolates to $C_{36}H_{74}$ and generally agrees with data within $0.05 \cdot p^{1+g}$ (the estimated uncertainty), we believe that the equation may be extrapolated to $C_{43}H_{88}$ without introducing large systematic errors. Figure 22 supports this opinion. The work of Morgan and Kobayashi (1992) showed similar trends with the data of Mazee for $C_{43}H_{88}$. In both this work and that of Morgan and Kobayashi, the data of Mazee for the other systems ($C_{21}H_{44}$ through $C_{36}H_{74}$) appear to be of good quality, e.g., the seven data points for $C_{36}H_{74}$ have an average absolute deviation of $0.026 \cdot p^{1+g}$ calculated from Eq. (12).

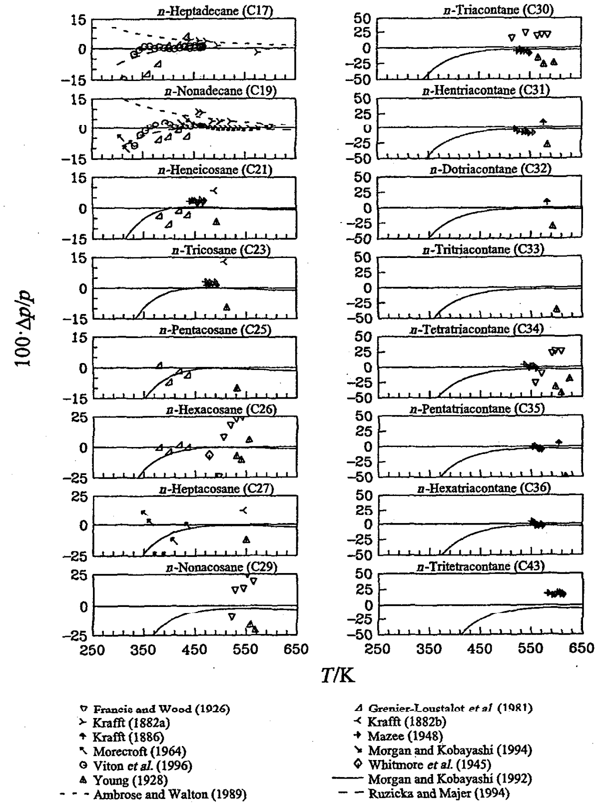

FIG. 22. Percent deviations of experimental vapor pressures from values obtained from Eq. (12) for (1) n-heptadecane, (2) n-nonadecane, (3) n-heneicosane, (4) n-tricosane, (5) n-pentacosane, (6) n-hexacosane, (7) n-heptacosane, (8) n-nonacosane, (9) n-triacontane, (10) n-hentriacontane, (11) n-dotriacontane, (12) n-tritriacontane, (13) n-tetratriacontane, (14) n-pentatriacontane, (15) n-hexatriacontane, and (16) n-tritetracontane.

At pressures below the range of most available data for $n>20$, the equation of Morgan and Kobayashi (1992) deviates, as shown in Figs. 21 and 22, substantially from our equation. There is little precise experimental evidence to support one equation or the other for $n>20$. However, as shown in Fig. 19, the equation of Morgan and Kobayashi deviates in a similar fashion from the data for n-decane for temperatures of 320 K and lower. For both n-decane and n-eicosane, our equation agrees well with that of Ambrose and Walton (1989) over all temperatures. For $n<10$, the de-

TABLE 7. Values of the vapor pressure estimated from the figure of Mazee (1948)

T/K	p^{1+g}/Pa	T/K	p^{1+g}/Pa
n-Heneicosane		*n*-Hentriacontane	
452.9	400.0	539.4	400.0
440.1	211.3	517.3	151.3
444.8	270.3	523.6	197.2
449.4	340.3	533.4	305.4
456.0	462.3	539.1	402.6
460.2	572.7	545.0	498.8
465.5	720.9	553.4	716.0
468.4	827.8	*n*-Tetratriacontane	
n-Tricosane		558.6	400.0
472.7	400.0	537.1	160.3
470.6	369.7	545.0	221.3
476.2	473.0	549.5	278.5
478.0	522.3	552.5	316.9
484.0	679.1	555.3	361.3
488.5	835.4	559.3	418.7
492.1	959.2	*n*-Pentatriacontane	
n-Tetracosane		565.5	400.0
481.8	400.0	552.5	234.4
472.6	264.8	556.2	280.5
481.9	402.6	561.8	348.3
484.7	457.0	564.0	378.4
489.0	568.7	566.6	426.5
498.8	866.8	570.5	493.1
n-Octacosane		*n*-Hexatriacontane	
515.2	400.0	571.6	400.0
521.7	530.8	550.1	162.8
518.2	459.1	553.4	188.3
510.5	327.3	557.1	211.8
506.3	278.5	559.9	244.3
503.0	233.3	563.4	281.8
498.3	187.9	567.6	345.1
493.6	153.1	*n*-Tritetracontane	
n-Triacontane		605.2	400.0
531.7	400.0	580.8	134.2
523.6	278.5	589.3	195.4
529.1	368.9	594.6	248.3
532.8	424.5	599.6	323.5
537.7	518.7	604.3	398.9
544.7	696.5	608.7	473.0
548.0	776.1	611.7	524.7

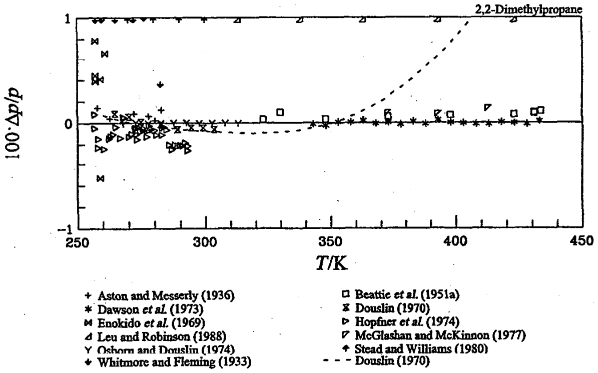

FIG. 23. Percent deviations of experimental vapor pressures from values obtained from Eq. (27) for 2,2-dimethylpropane.

viations calculated from Morgan and Kobayashi are substantially higher than those from this model and that of Ambrose and Walton.

7. Acknowledgments

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