Liquid Densities at Elevated Pressures of *n*-Alkanes from C_5 to C_{16}: A Critical Evaluation of Experimental Data

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The published experimental data for *n*-alkanes are critically reviewed and the parameters of the Tait equation are given. This equation allows the calculation of smoothed values of liquid density of *n*-alkanes from pentane to hexadecane over a temperature and pressure range.

Introduction

The work, the results of which are summarized here, is a continuation of the critical evaluation of published $-\rho-T$ data in a liquid state for two groups of substances, 1-alkanols and *n*-alkanes. The critical evaluation of the published density data obtained at atmospheric pressure or along a saturation curve for 1-alkanols and *n*-alkanes was performed and published [93-cib] as a part of the IUPAC Project on Vapor-Liquid Equilibria in 1-Alkanol + -Alkane Mixtures [94-dym] followed by the paper on densities of 1-alkanols at elevated pressures [94-cib/zik]. In this paper published densities for liquid *n*-alkanes from pentane to hexadecane at pressures higher than either 0.1 MPa or the saturation pressure are reviewed and critically evaluated.

Sources of Data

The original experimental data (8484 data points) processed were extracted from a source database developed and installed under the FOXPRO 2.5 environment in the laboratory of the authors. The database contains published experimental data for several properties of pure liquids (density, volume, compression, compressibilities, expansivities, compressibility factor, speed of sound) as a function of temperature and pressure along with a large amount of auxiliary information compiled from the literature.

The characteristics of data that were available in the database for density and related quantities (molar and specific volumes, volume or density ratios, compression) of -alkanes are summarized in Table 1. The displayed temperature ranges and numbers of experimental values are restricted up to the critical temperature (for the critical temperatures selected see [93-cib]); i.e., only subcritical liquid density data were taken from the source database.

Treatment of Data and Method of Data Evaluation

The procedures of treatment of data and the critical evaluation were essentially the same as those employed for 1-alkanols, and the details may be found in our previous paper [94-cib/zik]. Therefore a brief summarization only is given below.

Available experimental data on the compressed liquid density of alkanes were fitted by a Tait equation with temperature dependent parameters *C(T)* and *B(T)* written in the form

$$\rho(T,P,\vec{c},\vec{b}) = \frac{\rho(T,P_{\mathrm{ref}}(T))}{1 - C(T,\vec{c})\ln\left[\dfrac{B(T,\vec{b}) + P}{B(T,\vec{b}) + P_{\mathrm{ref}}(T)}\right]} \quad (1)$$

where

$$C(T,\vec{c}) = \sum_{i=0}^{N_C} c_i[(T - T_0)/100]^i \qquad \vec{c} = \{c_i\} = \{c_0, ..., c_{N_C}\} \quad (2)$$

$$B(T,\vec{b}) = \sum_{i=0}^{N_B} b_i[(T - T_0)/100]^i \qquad \vec{b} = \{b_i\} = \{b_0, ..., b_{N_B}\} \quad (3)$$

and T_0 is a parameter with a preselected fixed value for which $C(T_0) = c_0$ and $B(T_0) = b_0$ hold. The reference lines, $\rho(T,P_{\mathrm{ref}}(T))$ and $P_{\mathrm{ref}}(T)$, were selected in the same way as for 1-alkanols; i.e., at temperatures below the normal boiling temperature the densities at atmospheric pressure ($P_{\mathrm{ref}} = 0.101\ 325$ MPa) were used, while for higher temperatures the values along the saturation curve, i.e. saturated liquid densities and saturated vapor pressures, were employed. If the densities at atmospheric pressure or at saturation for the same sample were also reported along with compressed liquid density data, then those values were preferably used for the reference density, $\rho(T,P_{\mathrm{ref}})$. If the reference values were not available in the original source, then densities obtained from the critical evaluation [93-cib] were employed in the correlations. Saturated vapor pressures were calculated from the smoothing functions given by Ambrose and Walton [89-amb/wal].

Adjustable parameters $\vec{c}$ and $\vec{b}$ of function 1 were obtained by minimizing the objective function

$$\phi(\vec{c},\vec{b}) = \sum_{j=1}^{N_p} w_j[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]^2 \quad (4)$$

where ρ_j, T_j, P_j is the *j*th experimental data point, $\rho(T_j,P_j,\vec{c},\vec{b})$ is the value calculated from function 1 with parameters $\vec{c}$ and $\vec{b}$ for the values T_j and P_j, and N_p is the number of experimental values of density taken into the correlation. Adjustable parameters were calculated by the Marquardt algorithm in double precision to minimize the influence of rounding errors. Statistical weights, w_j, in eq 4, defined as

$$w_j = \mu_j/(\delta\rho_j)^2 \quad (5)$$

where $\delta\rho_j$ is the experimental uncertainty taken from the source database and either given by the authors (preferably) or estimated by a compiler for the *j*th density value in a correlated data set, were adjusted by varying the parameter μ_j ($\mu_j = 0$ for rejected data points). The calculations of the parameters $\vec{c}$ and $\vec{b}$ were repeated until the final fit was obtained where the deviations between

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S0021-9568(96)00058-1 CCC: $12.00

Table 1. Characteristics of Data Sets: Overall Number of Data Points, N_p, Temperature and Pressure Ranges within the Liquid State, T_{min}, T_{max}, P_{min}, and P_{max}, Experimental Method Used, Types of Data, and Purities of Measured Samples

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
				Pentane (CASRN 109-66-0)				
31-bri	30	273.15	368.15	98.2	980.8	vb	D	
35-sag/lac	84	294.26	377.59	0.7	20.7	nd	D	99.3[d]
42-sag/lac	147	310.93	444.26	0.1	68.9	vl	D	99.7m[d]
53-li/can	36	373.15	448.15	1.1	22.1	nd	D	99.88m[d]
69-bra/fre	9	303.15	303.15	50.0	450.0	vb	D	
74-hou	12	295.15	295.15	200.0	2400.0	vs	D	
77-aft/zaw	13	353.17	403.35	0.6	4.0	vl	D[h]	99.96w[e]
79-geh/len	31	273.15	423.15	5.0	50.0	vs/ia	S	
79-geh/len	107	295.15	463.15	3.2	228.6	vs/ia	D	
80-sca/lyo	143	248.15	373.15	0.5	284.5	vb	D	>99.5[d]
84-vas	143	173.15	448.15	0.6	148.3	pi	D	99.9w[e]
85-kra/mue	88	238.37	465.24	0.7	60.6	ia	D[h]	>99.96m[e]
86-gri/kur	7	453.21	469.02	3.1	4.6	pi	D	99.9w[e]
87-eas/woo	28	278.15	338.15	10.0	60.0	vb	S	>99.0[d]
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[h]	99.6m[e]
87-hol/goe-1[k]	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.8m[e]
92-kir/len	139	318.00	443.00	7.5	70.3	vs	D	>99[d]
total	1027	173.15	469.02	0.1	2400.0			
				Hexane (CASRN 110-54-3)				
31-bri	27	273.15	368.15	98.2	1078.8	vb	D	
40-kel/fel	44	373.15	498.15	0.6	31.6	pi	D	
51-edu/new	40	273.15	333.15	50.7	506.6	vl	D[f]	
54-ste/sag	78	310.93	477.59	0.7	67.3	vl	D[g]	>99.5m[d]
57-wal/ric	2	292.15	305.15	4150.0	9570.0	sw	D	
67-mop	38	223.15	298.15	10.2	202.8	vb	D	>98[d]
69-bra/fre	9	303.15	303.15	50.0	450.0	vb	D	
70-erm/skr	58	495.55	504.35	2.6	3.5	nd	D	
70-kus/tas	20	298.15	353.15	39.2	196.1	vl	D	
72-gol/ada	30	303.15	393.15	50.7	253.3	vb	D	
72-lys	2	297.15	297.15	139.0	328.0	sw	D	
76-ras/gri	222	223.15	473.15	2.4	150.6	pi	D	
76-ta'	102	298.15	473.15	50.0	500.0	cl	D	
78-gou	90	295.15	394.65	5.1	40.1	vl	D	
78-tak	12	283.15	333.15	55.3	103.5	ul[i]	C	
78-tak	12	283.15	333.15	55.3	103.5	ul[i]	C	
79-dic	19	295.00	295.00	1500.0	37000.0	sw	D	99[d]
79-dym/you	27	298.15	373.15	48.5	564.0	vb	D	99.7m[e]
79-isd/dym	4	298.15	348.15	10.0	20.0	ul	D	>99[e]
79-isd/dym	12	298.15	348.15	50.0	500.0	vb	D	>99[e]
80-sca/lyo	146	248.15	373.15	14.8	253.3	vb	D	>99.96m[d]
82-kob/nis	4	298.15	298.15	49.0	196.1	vs	D	
82-kur/gri	65	498.15	507.85	2.9	11.0	pi	D	99.93w[e]
83-kur/gri	28	498.15	498.15	3.0	124.1	pi	D	99.93[e]
85-mak	72	298.15	333.15	7.4	111.8	nd	D	
85-tak/ter	2	298.15	298.15	50.0	100.0	vb	D	
85-zaw	17	398.15	448.15	0.7	4.2	nd	D	99.88w[d]
87-hol/goe-1[l]	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.8m[e]
87-led	70	298.15	358.15	10.0	330.0	vb	D	99.5[d]
88-mor/aon	71	298.15	313.15	3.2	145.6	vl	D	
91-mel/mel	105	293.15	413.15	10.0	500.0	pi	D	
91-orm/dak	9	298.15	298.15	2.0	33.8	mo	D	99.0[d]
92-kir/len	76	313.00	448.00	0.2	65.9	vs	D	>99[d]
92-sus/bud	50	294.35	294.35	0.8	34.6	mo	D	99.2[e]
95-sau/hol	36	263.15	353.15	1.0	10.0	mo	D[h]	99.63[e]
95-sau/hol	36	317.60	472.95	1.9	49.8	ia	D[h]	99.63[e]
total	1640	223.15	507.85	0.2	37000.0			
				Heptane (CASRN 142-82-5)				
31-bri	28	273.15	368.15	49.1	1078.8	vb	D	
37-smi/bea	46	303.15	523.15	0.7	35.6	nd	D[f]	
49-bri	11	298.15	298.15	49.0	980.7	vs	D	
51-edu/new	40	273.15	333.15	50.7	506.6	vl	D	
55-nic/rea	111	277.59	510.93	0.1	69.1	vl	D	99.94m[d]
60-boe	59	273.15	393.15	9.9	117.8	vb	D	99.2m[d]
64-doo	60	303.15	523.15	5.0	500.0	vl	S	
66-ata	30	286.15	343.15	101.3	1013.3	vb	D	
69-bra/fre	8	303.15	303.15	50.0	400.0	vb	D	
70-kus/tas	20	298.15	353.15	39.2	196.1	vl	D	
72-gol/ada	30	303.15	393.15	50.7	253.3	vb	D	
78-tak	12	283.15	333.15	55.3	103.5	ul[i]	C	
78-tak	12	283.15	333.15	55.3	103.5	ul[i]	C	
80-oza/ooy	42	298.20	348.20	9.9	196.2	vl	D	99.9m[e]
80-sca/lyo	189	248.15	373.25	0.7	200.1	vb	D	>99.9[d]
82-bac/eas	7	298.15	298.15	25.0	250.0	vb	D	

Table 1. (Continued)

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
				Heptane (CASRN 142-82-5) (Continued)				
82-zaw/vej	18	423.15	523.15	0.4	5.3	nd	D	99.99w[d]
85-mak	71	298.15	348.15	7.2	111.6	nd	D	
85-mur/tra	206	198.25	310.65	10.1	263.4	ul	C[g]	
85-vas	230	188.15	523.15	0.3	147.5	pi	D	99.9w[e]
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.8m[e]
87-hol/goe-1[k]	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.6m[e]
88-dym/mal	10	298.15	298.15	4.9	240.2	vb	D	99.5m[d]
88-dym/mal	17	298.15	310.65	5.2	271.1	vb	D	99.5m[d]
89-bet/pal	8	302.51	302.51	15.5	94.9	mo[j]	D	
89-bet/pal	8	302.51	302.51	15.5	94.9	mo[j]	D	
89-tos/fig	88	298.15	373.15	1.0	100.0	bu	D	99.9w[d]
91-kan/lag	12	313.15	353.15	10.0	40.0	mo	D	>99[d]
91-mal/woo	134	278.15	338.15	2.5	394.3	vb	D	99.994a[e]
91-pap/zia	9	298.15	298.15	2.0	33.8	mo	D	99.5[d]
92-sus/bud	50	294.35	294.35	0.8	34.6	mo	D	99.8[e]
total	1576	188.15	523.15	0.1	1078.8			
				Octane (CASRN 111-65-9)				
31-bri	22	273.15	368.15	49.1	980.8	vb	D	
42-fel/wat	89	373.15	548.15	0.5	30.4	nd	D	
49-bri	10	298.15	298.15	49.0	490.3	vs	D	
51-edu/new	36	273.15	333.15	50.7	506.6	vl	D	
60-boe	47	303.15	393.15	9.9	117.8	vb	D	99.9m[d]
69-bra/fre	8	303.15	303.15	50.0	400.0	vb	D	
71-ben/win	70	258.15	258.15	0.4	148.4	vb	D[g]	99.92m[d]
72-gol/ada	30	303.15	393.15	50.7	253.3	vb	D	
78-gou	66	293.15	393.15	2.5	40.5	vl	D	
78-tak	12	283.15	333.15	55.3	103.5	ul[i]	C	
78-tak	12	283.15	333.15	55.3	103.5	ul[i]	C	
80-sca/lyo	191	248.15	373.35	4.9	196.2	vb	D	>99.81m[d]
82-dym/rob	25	298.03	348.14	20.2	479.5	vb	D	99.5m[d]
85-mak	78	298.15	348.15	7.1	111.4	nd	D	
85-tak/ter	2	298.15	298.15	50.0	100.0	vb	D	
90-won/hay	18	298.20	348.20	0.7	6.9	mo	D	99[d]
91-ban/gar	55	318.15	373.15	1.0	10.0	mo	D[h]	98.8m[e]
91-dix/far	19	298.15	323.15	7.9	103.0	mo/bu	D	99.9[d]
91-tan/hos	16	298.15	348.15	9.9	151.0	va	D	98.0[e]
92-kir/len	47	323.00	448.00	8.0	66.5	vs	D	>99[d]
total	853	248.15	548.15	0.4	980.8			
				Nonane (CASRN 111-84-2)				
53-car/sag	88	310.93	510.93	0.2	69.2	vl	D[g]	99.6m[d]
60-boe	48	303.15	393.15	9.9	117.8	vb	D	99.2m[d]
64-doo	66	303.15	573.15	5.0	500.0	vl	S	
78-gri/lin	502	303.15	423.15	20.0	800.0	vl	D	99.79[e]
80-sca/lyo	160	248.15	373.15	2.0	301.2	vb	D	>99.5[d]
91-ban/gar	60	313.15	373.15	1.0	10.0	mo	D[h]	99.8m[e]
total	924	248.15	573.15	0.2	800.0			
				Decane (CASRN 124-18-5)				
31-bri	17	273.15	368.15	49.1	784.6	vb	D	
40-sag/lav	55	294.26	394.26	1.7	24.1	vl	D[f]	
42-rea/old	217	310.93	510.93	1.4	68.9	vl	S	
49-bri	6	298.15	298.15	49.0	294.2	vs	D	
70-sny/win	112	298.15	358.15	2.0	655.9	vb	D[g]	
78-gou	66	293.15	393.15	2.5	40.5	vl	D	
80-sca/lyo	61	248.15	373.25	14.8	294.3	vb	D	>99m[d]
82-dym/rob	16	298.31	373.11	36.8	420.2	vb	D	>99m[d]
83-geh/len	221	313.15	613.15	0.2	266.2	vs/ia	D	99.5m[e]
84-cul/mat	4	303.56	310.94	6.9	20.6	mo	D[h]	99.1m[e]
85-mak	75	298.15	348.15	7.1	111.1	nd	D	
85-tak/ter	2	298.15	298.15	50.0	100.0	vb	D	
86-gat/woo	18	298.14	399.81	0.2	20.5	mo	D	99.4m[d]
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.7m[e]
87-hol/goe-1[k]	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.7m[e]
91-ban/gar	60	313.15	373.15	1.0	10.0	mo	D[h]	98.9m[e]
92-sus/bud	50	294.35	294.35	0.8	34.6	mo	D	99.6[e]
total	990	248.15	613.15	0.2	784.6			
				Undecane (CASRN 1120-21-4)				
64-doo	70	303.15	573.15	5.0	500.0	vl	S	
80-lan/wur	148	258.25	313.25	10.0	300.0	vs	D	
total	218	258.25	573.15	5.0	500.0			
				Dodecane (CASRN 112-40-3)				
49-bri	3	298.15	298.15	49.0	147.1	vs	D	
58-cut/mcm	70	310.95	408.15	34.5	689.1	vb	D	

Table 1. (Continued)

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
				Dodecane (CASRN 112-40-3) (Continued)				
60-boe	24	303.15	393.15	9.9	117.8	vb	D	99.2m[d]
70-sny/win	92	298.15	358.15	1.7	416.9	vb	D[g]	
78-gou	90	298.15	393.75	5.1	40.1	vl	D	
80-lan/wur	88	268.45	313.25	10.0	250.0	vs	D	
82-dym/rob	31	298.19	373.26	17.1	441.9	vb	D	99m[d]
83-rou/ric	15	323.10	423.10	2.1	30.6	vb/cs	D	99[d]
85-eas/woo	12	298.27	323.35	25.0	150.0	vb	S	
85-mak	67	298.15	348.15	7.2	111.2	nd	D	
85-tak/ter	2	298.15	298.15	50.0	100.0	vb	D	
91-tan/hos	18	298.15	348.15	19.5	150.8	va	D	99.0[e]
total	512	268.45	423.10	1.7	689.1			
				Tridecane (CASRN 629-50-5)				
64-doo	70	303.15	573.15	5.0	500.0	vl	S	
				Tetradecane (CASRN 629-59-4)				
70-sny/win	113	298.15	358.15	0.9	366.8	vb	D[g]	
78-gou	90	298.15	393.35	5.1	40.1	vl	D	
85-tak/ter	1	298.15	298.15	50.0	50.0	vb	D	
87-hol/goe-1[l]	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.5[d]
total	209	293.15	393.35	0.9	366.8			
				Pentadecane (CASRN 629-62-9)				
58-cut/mcm	63	310.95	408.15	34.5	654.6	vb	D	
				Hexadecane (CASRN 544-76-3)				
60-boe	40	303.15	393.15	9.9	117.8	vb	D	99.2m[d]
70-sny/win	88	298.15	358.15	0.4	290.2	vb	D[g]	
78-gou	75	314.75	392.15	5.1	40.1	vl	D	
79-dym/you	23	298.15	373.15	12.0	450.5	vb	D	99.6m[e]
85-gla/pet	63	303.15	360.15	2.0	17.7	vl	D[h]	99.9m[e]
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[h]	>99[d]
87-hol/goe-1[k]	5	293.15	293.15	2.0	10.0	mo	D[h]	>99[d]
87-mat/rod	10	323.15	564.15	1.4	3.5	xx	D	99m[e]
91-ban/gar	60	318.15	373.15	1.0	10.0	mo	D[h]	99.4m[e]
91-tan/hos	13	298.15	348.15	9.9	150.5	va	D	98.0[e]
total	382	293.15	564.15	0.4	450.5			

Method used for measurements: bu, buoyancy method; cb, constant-volume cell with bellows; cl, constant-volume cell with liquid piston; ia, isochoric apparatus; mo, mechanical oscillator method; mo/bu, a combination of a vibrating-wire method with a buoyancy principle; nd, not described or stated in the reference; pi, piezometer of unspecified type; sw, shock wave method; ul, ultrasound velocity method; va, Aime method; vb, variable-volume cell with bellows; vb/cs, combination of vb cell with external solid piston syringe; vl, variable-volume cell with liquid piston; vs, variable-volume cell with solid piston; vs/ia, vs cell used in isochoric mode; xx, other methods. For the classification and description of the methods, see ref 85-tek/cib. [b] D, direct experimental data; S, smoothed data; C, densities calculated from ultrasound velocities. [c] No letter, unspecified percent; a, mass percent assuming water as an impurity; m, mole percent; w, mass percent. [d] Purity of source material is given only. [e] Final purity of the sample. [f] ITS-27 declared by the researchers. [g] ITS-48 declared by the researchers. [h] IPTS-68 declared by the researchers. [i] Two density data sets calculated from the same measured sound velocities by a classical integration and by a modified procedure, respectively. [j] Two data sets evaluated by absolute and relative methods, respectively. Same data are presented in ref 86-hol/goe. [l] Same data are presented in refs 86-hol/goe and 87-hol/goe.

retained experimental and smoothed values were roughly equal to the modified experimental uncertainties, $\delta\rho_j/\mu_j^{1/2}$, i.e., where the weighted standard deviation of the fit, s_w (see below), was close to unity.

Results

The results are summarized in Tables 2 and 3. Table 2 records the values of the parameters of eq 1 for each alkane along with some statistical information of the fits defined as follows:

$$\mathrm{RMSD} = \{\sum_{j=1}^{N_p}[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]^2/N_p\}^{1/2} \quad (6)$$

$$\mathrm{RMSD_r}/\% = 100\{\sum_{j=1}^{N_p}[1 - \rho(T_j,P_j,\vec{c},\vec{b})/\rho_j]^2/N_p\}^{1/2} \quad (7)$$

$$\mathrm{bias} = \sum_{j=1}^{N_p}[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]/N_p \quad (8)$$

$$\pm = \sum_{j=1}^{N_p}\mathrm{sign}[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]\cdot 1 \quad (9)$$

$$s_w = [\phi/(N_p - N_C - N_B - 2)]^{1/2} \quad (10)$$

where N_p is the overall number of experimental data points retained for the correlation. Temperature and pressure ranges of validity of the fits given in the table are informative only and allow one to avoid extrapolation using eq 1 with the parameters from Table 2 beyond $P-T$ areas shown in the figures (Figure 1). That plot provides crude information on the distribution of the retained data points in the $P-T$ area for each fit performed.

Table 3 summarizes some statistical information derived from the fits. Only those data subsets for which the temperature and pressure ranges are displayed in the table were retained in the correlations. The statistical characteristics of these subsets refer only to the data points retained in the correlation. On the other hand, the characteristics of the rejected data subsets, i.e. those for which no T and P ranges are given in the table, illustrate the deviations of the rejected data points from eq 1, but

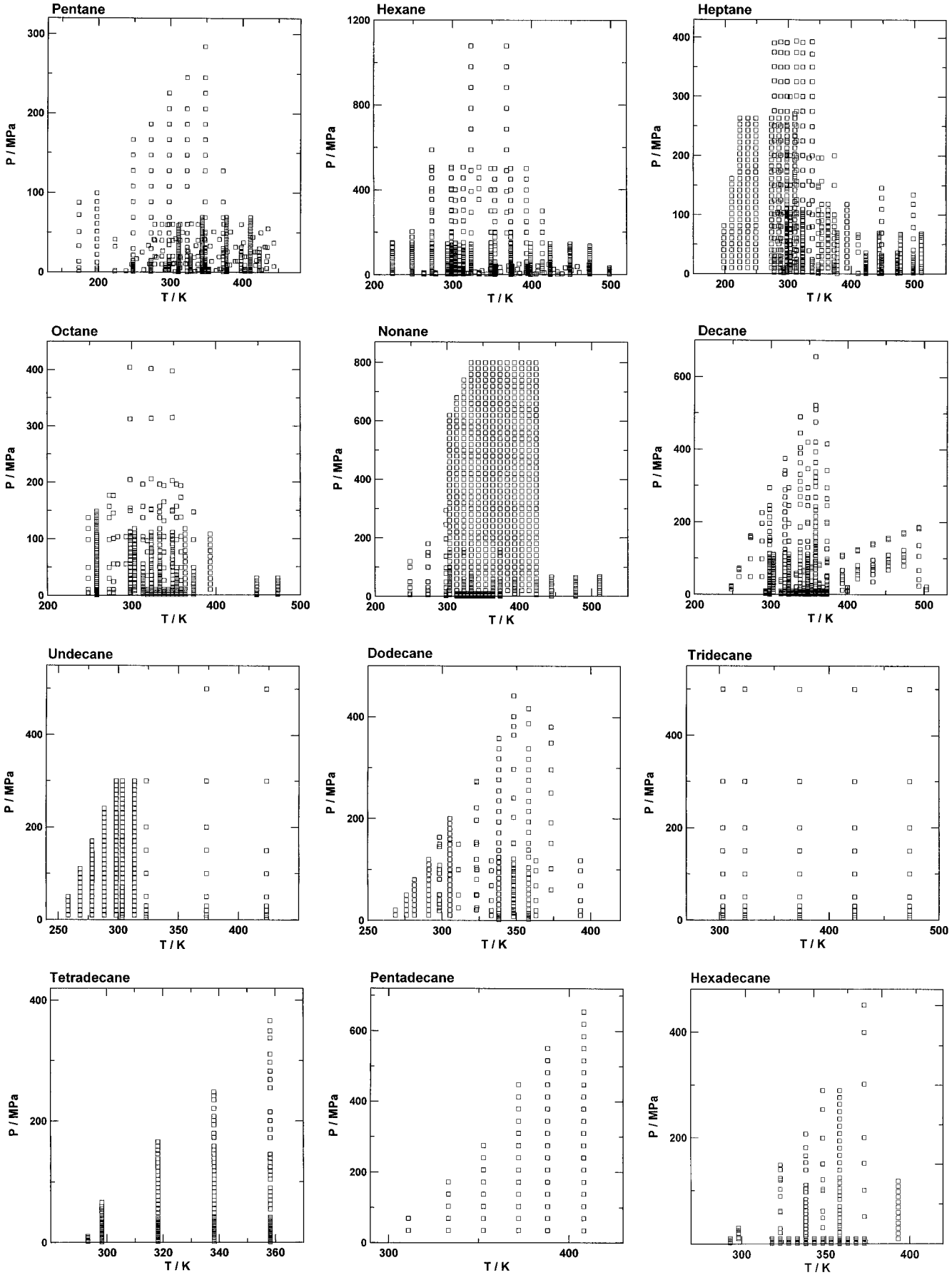

Figure 1. Temperature and pressure coordinates of data points retained for the correlations.

only for those values within $T-P$ areas of the retained data (see Figure 1); thus N_p and the characteristics correspond to the rejected data points within the $T-P$ ranges of the fits.

Table 2. Parameters c_i, b_i, and T_0 of Eq 1, Temperature and Pressure Ranges,[a] T_{min}, T_{max}, P_{min}, and P_{max}, Absolute, RMSD, and Relative, $RMSD_r$, Root Mean Square Deviations, Biases, bias, Number of Data Points, N_p, ±, and Weighted Standard Deviations, s_w

	pentane	hexane	heptane	octane		pentane	hexane	heptane	octane
c_0	0.088 843	0.092 380	0.091 609	0.092 825	T_{max}/K	443.53	498.15	510.93	473.15
c_1/K^{-1}	−0.003 788	−0.004 522	−0.001 099	−0.005741	P_{min}/MPa	0.14	0.57	0.18	0.42
c_2/K^{-2}			−0.001 513		P_{max}/MPa	284.50	1078.83	394.34	404.10
b_0/MPa	35.8259	56.0622	64.0193	73.8539	RMSD/kg·m^{-3}	0.770	0.693	0.933	0.477
b_1/MPa·K^{-1}	−44.2380	−56.5365	−53.4677	−61.7706	$RMSD_r$/%	0.121	0.112	0.153	0.069
b_2/MPa·K^{-2}	17.7963	18.6982	15.7048	24.6982	bias/kg·m^{-3}	0.071	−0.033	0.177	−0.048
b_3/MPa·K^{-3}	−5.7066	−2.9566	−3.9551	−13.7438	N_p	509	796	738	517
b_4/MPa·K^{-4}	1.4456	0.2334	0.8103	4.2338	±	77	52	46	41
T_0/K	310.93	298.15	298.15	298.15	s_w	0.981	0.955	1.030	0.820
T_{min}/K	173.15	223.15	198.25	248.15					

	nonane	decane	undecane	dodecane		nonane	decane	undecane	dodecane
c_0	0.094 316	0.087 992	0.090 328	0.090 545	T_{max}/K	510.93	503.15	423.15	393.15
c_1/K^{-1}	−0.002 960	−0.000 816	−0.001 105		P_{min}/MPa	0.60	0.20	5.00	2.03
b_0/MPa	63.4470	83.5746	83.6261	90.6028	P_{max}/MPa	800.00	655.88	500.00	441.90
b_1/MPa·K^{-1}	−54.0094	−61.9418	−44.4334	−58.5280	RMSD/kg·m^{-3}	0.468	0.745	0.344	0.666
b_2/MPa·K^{-2}	17.5175	21.8935	58.8378	70.5209	$RMSD_r$/%	0.064	0.102	0.044	0.083
b_3/MPa·K^{-3}	−3.9433	−6.4316	−132.7102	−117.9246	bias/kg·m^{-3}	0.031	−0.056	0.046	0.052
b_4/MPa·K^{-4}	0.6272	1.0545	69.7765	63.1006	N_p	692	439	181	201
T /K	333.15	294.35	298.25	298.15	±	0	−37	11	39
/K	248.15	248.15	258.25	268.45	s_w	0.951	0.847	1.001	0.938

	tridecane	tetradecane	pentadecane[b]	hexadecane		tridecane	tetradecane	pentadecane[b]	hexadecane
	0.087 988	0.090 131	0.088 503	0.090 512	P_{min}/MPa	5.00	0.89	34.46	0.39
/MPa	89.5217	78.3594	51.7990	73.9549	P_{max}/MPa	500.00	366.80	654.64	450.50
/MPa·K^{-1}	−56.5397	−49.2510	−35.3533	−47.6742	RMSD/kg·m^{-3}	0.630	0.313	0.389	0.368
/MPa·K^{-2}	10.0334		12.5370	20.6979	$RMSD_r$/%	0.080	0.040	0.048	0.047
/MPa·K^{-3}				26.0659	bias/kg·m^{-3}	0.112	0.022	0.010	0.045
/K	303.15	338.15	408.15	358.15	N_p	50	179	63	171
/K	303.15	293.15	310.95	293.15	±	16	7	−9	−5
/K	473.15	358.15	408.15	393.15	s_w	1.059	1.043	0.960	0.944

The low limit of pressure ranges is 0.1 MPa or a saturation pressure (whichever is higher) for all fits; P_{min} is the lowest pressure in a particular set of compressed liquid density data retained for the corelation. [b] See discussion in Results.

Data points at high temperatures of some retained data sets were rejected in those cases where deviations from the Tait equation exceeded 10 kg·m^{-3} and it was not possible to improve the fit by additional parameters b_i and c_i. Thus $P-T$ ranges of some fits do not cover the entire original range of retained data sets. There might be several reasons for those large deviations; lower accuracy of data and systematic errors in measured variables at very high temperatures and pressures, decomposition of the substance at high temperatures, a poorer performance of the Tait equation in the vicinity of the gas−liquid critical point, and at last a reason discussed below.

In several cases an inconsistency of the data at high temperatures with those at lower temperature ranges was noticed by examining the shape of the temperature dependence of the Tait parameter $B(T,\vec{b})$. Since the temperature dependence of the parameter $C(T,\vec{c})$ is moderate (if any, see Table 2), the temperature dependence of isothermal compressibility derived from the Tait equation is determined mainly by the temperature dependence of the parameter $B(T,\vec{b})$. Therefore the function $B(T,\vec{b})$ should be a decreasing function of temperature to describe the increase of isothermal compressibility with increasing temperature along an isobar and no local minimum should appear on it to avoid a maximum in isothermal compressibility. The local minima on $B(T,\vec{b})$ were observed for undecane (around 460 K) and hexadecane (around 410 K) when the correlations were performed in temperature ranges as wide as possible. Therefore the data at high temperatures for these two alkanes were also rejected. The examination of the function $B(T,\vec{b})$ of the final fits (Table 2) reveals that this function decreases as either a straight line or a convex function of increasing temperature without any inflection point for most of the fits (pentane through decane, tridecane through pentadecane), while one or two inflection points were observed for the other alkanes, i.e., for hexadecane around 330 K (the function is slightly concave, being close to the straight line at lower temperatures), for undecane around 320 K and 380 K, and for dodecane around 325 K and 365 K (the functions $B(T,\vec{b})$ are slightly concave between these temperatures for the last two alkanes with the effect being more pronounced in the case of undecane). The inflection points on the $B(T,\vec{b})$ function signal the mutual inconsistency of data taken for the correlation. It can be clearly seen in the case of undecane where two data sets with slightly overlapping temperature ranges were available (see Tables 1 and 3). When the Tait equation was fit to each data set alone, good fits with $N_C = 0$ and $N_B = 2$ but with different values of parameters c_i and b_i were obtained, while a larger number of parameters c_i and b_i was required to achieve a good fit when both data sets were correlated together. Consequently, the inflection points and even a minimum (see above) on the function $B(T,\vec{b})$ appeared. Since the smoothed values reported by Doolittle [64-doo] at temperatures above the normal boiling point are based on a hypothetical specific volume at zero pressure, the data from this source up to temperatures close to the normal boiling point were retained in the correlations (this holds also for heptane, nonane, and tridecane) while those at higher temperatures were rejected. Moreover, the saturated liquid densities obtained by tentative interpolations between Doolittle's values at P = (0, 5, and 10) MPa using the Hudleston equation (used by Doolittle to smooth the data) did not show a good agreement with the reference line [93-cib]. However, even after the values in a high-temperature range were rejected, the effect of the inconsistency remained, causing the inflection points. Thus the inflection points observed on the $B(T,\vec{b})$ curve for the above men-

Table 3. Statistical Characteristics of Individual Data Sets for the Fits in Table 2: Temperature and Pressure Ranges Taken into the Correlations, T_{min}, T_{max}, P_{min}, and P_{max}, Absolute, RMSD, and Relative, $RMSD_r$, Root Mean Square Deviations, Biases, bias, Number of Data Points, N_p, ±, and Origin of the Reference Density Values Used in the Correlations, RD[a]

ref	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	RMSD/kg·m^{-3}	$RMSD_r$/%	bias/kg·m^{-3}	N_p	±	RD[a]
					Pentane					
31-bri					7.162	0.999	6.895	6	6	(o)
35-sag/lac	310.93	377.59	0.7	20.7	0.592	0.097	0.262	56	28	o
42-sag/lac	310.93	410.93	0.1	68.9	0.768	0.124	0.083	118	50	(o)
53-li/can					1.529	0.296	0.104	27	−1	(o)
69-bra/fre					1.818	0.255	0.421	5	1	o
74-hou					1.986	0.270	−1.986	1	−1	o
77-aft/zaw	353.17	403.35	0.6	4.0	1.000	0.178	0.725	12	12	o
79-geh/len					7.026	1.125	6.857	31	31	e
79-geh/len					13.851	2.092	8.884	89	87	e
80-sca/lyo	248.15	373.15	0.5	284.5	0.812	0.120	0.070	134	6	(o)
84-vas	173.15	423.15	0.6	99.5	1.068	0.165	0.333	76	54	e
85-kra/mue	238.37	443.53	0.7	60.6	0.353	0.064	−0.193	75	−53	e
86-gri/kur								0	0	e
87-eas/woo	278.15	338.15	10.0	60.0	0.772	0.123	−0.609	28	−24	o
87-hol/goe	293.15	293.15	2.0	10.0	0.017	0.003	0.012	5	3	o
87-hol/goe-1	293.15	293.15	2.0	10.0	0.017	0.003	0.004	5	1	o
92-kir/len					6.929	1.186	−6.570	139	−139	e
					Hexane					
31-bri	273.15	368.15	98.2	1078.8	0.997	0.121	0.343	27	11	(o)
40-kel/fel	373.15	498.15	0.6	31.6	1.261	0.276	−0.250	43	−15	e
51-edu/new	273.15	333.15	50.7	506.6	0.599	0.079	−0.194	34	−4	o
54-ste/sag					2.051	0.354	1.711	78	68	e
57-wal/ric								0	0	o
67-mop	223.15	298.15	10.2	202.8	0.414	0.056	0.016	38	6	o
69-bra/fre	303.15	303.15	150.0	400.0	0.491	0.063	−0.373	5	−5	o
70-erm/skr					2.764	0.713	2.394	18	12	e
70-kus/tas					1.353	0.192	−0.276	20	−6	(o)
72-gol/ada					10.570	1.507	−9.459	30	−30	o
72-lys					14.152	1.844	−13.958	2	−2	o
76-ras/gri	223.15	473.15	2.4	150.6	0.613	0.093	0.336	221	121	(o)
76-ta'					2.822	0.379	−1.154	102	−26	e
78-gou	354.15	394.65	5.1	40.1	0.307	0.049	0.077	45	−7	e
78-tak					9.944	1.364	8.263	12	12	e
78-tak					1.853	0.260	0.561	12	6	e
79-dic								0	0	e
79-dym/you					2.093	0.286	−1.674	27	−23	o
79-isd/dym	298.15	348.15	10.0	20.0	0.507	0.080	0.415	4	4	o
79-isd/dym	298.15	348.15	50.0	500.0	1.102	0.142	−0.895	11	−9	o
80-sca/lyo	248.15	373.15	14.8	253.3	0.849	0.118	−0.546	109	−65	(o)
82-kob/nis					1.585	0.213	1.522	4	4	o
82-kur/gri					2.768	0.674	2.560	9	9	e
83-kur/gri					9.646	1.612	−5.281	28	−8	e
85-mak	298.15	303.15	7.4	111.8	0.636	0.091	−0.616	34	−34	o
85-tak/ter	298.15	298.15	50.0	100.0	0.192	0.027	−0.161	2	−2	o
85-zaw	398.15	423.15	0.7	4.2	0.600	0.106	0.290	11	5	o
87-hol/goe-1	293.15	293.15	2.0	10.0	0.217	0.032	0.196	5	5	o
87-led					5.069	0.671	4.294	70	70	o
88-mor/aon	298.15	313.15	3.2	145.6	0.269	0.039	0.197	71	59	o
91-mel/mel	353.15	413.15	10.0	500.0	0.953	0.149	−0.159	55	−5	(o)
91-orm/dak	298.15	298.15	2.0	33.8	0.570	0.085	−0.541	9	−9	o
92-kir/len					3.842	0.665	−1.021	76	−8	e
92-sus/bud					1.061	0.156	0.998	50	50	o
95-sau/hol	263.15	353.15	1.0	10.0	0.178	0.027	0.138	36	30	(o)
95-sau/hol	317.60	472.95	1.9	49.8	0.506	0.089	−0.441	36	−34	e
					Heptane					
31-bri					3.795	0.479	3.545	14	14	(o)
37-smi/bea	423.15	473.15	0.7	35.6	1.441	0.241	1.034	19	19	e
49-bri					1.148	0.151	−1.052	8	−8	o
51-edu/new					1.369	0.170	1.011	28	20	o
55-nic/rea	377.59	510.93	0.2	69.1	2.403	0.415	1.943	59	51	e
60-boe	363.15	393.15	9.9	117.8	0.545	0.080	−0.417	24	−16	o
64-doo	303.15	323.15	5.0	300.0	0.353	0.050	0.272	18	12	o
66-ata					3.028	0.386	2.474	9	9	o
69-bra/fre					3.206	0.408	2.966	7	7	o
70-kus/tas	298.15	353.15	39.2	196.1	0.374	0.051	−0.048	20	−6	o
72-gol/ada					5.924	0.812	−3.714	30	−24	o
78-tak					1.203	0.164	−0.179	12	2	e
78-tak	283.15	333.15	55.3	103.5	0.288	0.040	0.152	11	5	e
80-oza/ooy					0.917	0.127	−0.063	42	−2	o
80-sca/lyo	348.05	373.25	0.7	200.1	0.592	0.086	0.043	49	19	(o)
82-bac/eas	298.15	298.15	25.0	250.0	0.248	0.032	0.182	7	5	o
82-zaw/vej	448.15	498.15	0.7	5.3	1.018	0.198	0.175	8	2	o
85-mak	298.15	323.15	7.2	110.7	0.282	0.039	0.060	55	5	o

Table 3. (Continued)

ref	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	RMSD/kg·m^{-3}	RMSD$_r$/%	bias/kg·m^{-3}	N_p	±	RD[a]
					Heptane (Continued)					
85-mur/tra	198.25	310.65	10.1	263.4	0.243	0.031	0.019	206	−24	o
85-vas	423.15	498.15	0.6	145.5	1.441	0.230	0.530	67	19	(o)
87-hol/goe	293.15	293.15	2.0	10.0	0.114	0.016	0.097	5	5	o
87-hol/goe-1	293.15	293.15	2.0	10.0	0.114	0.016	0.097	5	5	o
88-dym/mal					0.970	0.128	−0.815	10	−10	o
88-dym/mal	298.15	310.65	5.2	271.1	0.702	0.090	0.359	17	7	o
89-bet/pal					0.908	0.128	−0.766	8	−8	o
89-bet/pal	302.51	302.51	15.5	94.9	0.428	0.060	−0.068	7	−1	o
89-tos/fig	353.15	373.15	10.0	100.0	0.657	0.097	−0.275	27	−7	(o)
91-kan/lag					2.907	0.431	−2.749	12	−12	o
91-mal/woo	278.15	338.15	2.5	394.3	0.557	0.072	−0.345	134	−54	(o)
91-pap/zia					0.686	0.098	−0.613	9	−9	o
92-sus/bud					0.888	0.127	0.846	50	50	o
					Octane					
31-bri					1.557	0.201	0.765	13	5	(o)
42-fel/wat	448.15	473.15	0.5	30.4	1.044	0.188	0.481	23	3	e
49-bri					2.667	0.336	−2.652	8	−8	o
51-edu/new					2.851	0.359	−2.218	27	−27	o
60-boe	303.15	393.15	9.9	117.8	0.223	0.031	0.035	46	12	o
69-bra/fre					2.131	0.270	−2.070	8	−8	o
71-ben/win	258.15	258.15	0.4	148.4	0.549	0.071	−0.193	70	−6	o
72-gol/ada					7.020	0.905	−2.975	30	2	o
78-gou	313.15	373.15	2.5	40.5	0.541	0.079	−0.080	44	−6	o
78-tak					1.210	0.161	−0.840	12	−8	e
78-tak	283.15	333.15	55.3	103.5	0.479	0.063	−0.330	12	−8	e
80-sca/lyo	248.15	373.35	4.9	196.2	0.503	0.067	−0.188	150	−2	(o)
82-dym/rob	298.03	348.14	20.2	404.1	0.742	0.096	0.199	21	5	o
85-mak	298.15	348.15	7.1	111.4	0.109	0.015	0.007	78	−2	o
85-tak/ter	298.15	298.15	50.0	100.0	0.150	0.020	0.144	2	2	o
90-won/hay					2.398	0.347	−1.056	18	−8	o
91-ban/gar	318.15	373.15	1.0	10.0	0.197	0.030	0.135	55	39	o
91-dix/far					1.683	0.230	1.459	19	17	o
91-tan/hos	298.15	348.15	9.9	151.0	0.245	0.032	−0.040	16	4	o
92-kir/len					10.823	1.713	−9.757	47	−47	e
					Nonane					
53-car/sag	444.26	510.93	0.6	67.6	0.932	0.146	0.332	28	8	e
60-boe	303.15	393.15	9.9	98.2	0.482	0.066	−0.282	30	−10	o
64-doo	303.15	423.15	5.0	500.0	1.038	0.144	0.473	35	21	(o)
78-gri/lin	303.15	423.15	20.0	800.0	0.339	0.044	0.039	502	−42	o
80-sca/lyo	248.15	298.15	2.1	294.3	0.801	0.102	−0.577	37	−21	(o)
91-ban/gar	313.15	373.15	1.0	10.0	0.142	0.021	0.104	60	44	o
					Decane					
31-bri					4.451	0.532	3.562	15	13	(o)
40-sag/lav					1.467	0.213	1.063	55	35	o
42-rea/old					4.424	0.642	3.825	186	170	o
49-bri	298.15	298.15	147.1	294.2	0.757	0.091	0.354	4	2	o
70-sny/win	298.15	358.15	2.0	655.9	0.611	0.079	−0.337	112	−58	o
78-gou					4.414	0.610	4.146	66	66	(o)
80-sca/lyo	248.15	373.25	14.8	294.3	0.917	0.116	0.465	61	27	(o)
82-dym/rob	298.31	373.11	36.8	420.2	1.286	0.157	−0.041	16	−6	o
83-geh/len	313.15	503.15	1.3	186.3	1.163	0.171	−0.174	84	−24	e
84-cul/mat					0.937	0.128	0.858	4	4	e
85-mak	298.15	348.15	7.1	111.1	0.158	0.021	0.006	75	5	o
85-tak/ter					4.733	0.610	4.727	2	2	o
86-gat/woo	298.14	399.81	0.2	20.5	0.343	0.051	−0.193	17	−7	e
87-hol/goe	293.15	293.15	2.0	10.0	0.146	0.020	0.129	5	5	o
87-hol/goe-1	293.15	293.15	2.0	10.0	0.146	0.020	0.129	5	5	o
91-ban/gar	313.15	373.15	1.0	10.0	0.138	0.020	0.016	60	14	o
92-sus/bud					0.826	0.111	0.776	50	50	o
					Undecane					
64-doo	303.15	423.15	5.0	500.0	0.456	0.061	0.216	33	11	(o)
80-lan/wur	258.25	313.25	10.0	300.0	0.313	0.039	0.008	148	0	o
					Dodecane					
49-bri					5.403	0.674	−5.065	3	−3	o
58-cut/mcm					5.554	0.685	−4.395	43	−37	o
60-boe	333.15	393.15	9.9	117.8	0.596	0.078	−0.180	18	0	o
70-sny/win	338.15	358.15	2.0	416.9	0.927	0.116	−0.008	56	0	o
78-gou					4.642	0.622	−2.709	75	−69	e
80-lan/wur	268.45	305.25	10.0	200.0	0.300	0.038	0.064	47	13	o
82-dym/rob	298.19	373.26	17.1	441.9	0.888	0.107	0.224	31	9	o
83-rou/ric					1.117	0.152	0.920	10	10	o
85-eas/woo	298.27	323.35	25.0	150.0	0.419	0.054	0.248	12	4	e
85-mak	348.15	348.15	7.6	111.2	0.321	0.042	−0.042	17	3	o
85-tak/ter	298.15	298.15	50.0	100.0	0.554	0.071	−0.552	2	−2	o

Table 3. (Continued)

ref	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	RMSD/kg·m^{-3}	RMSD$_r$/%	bias/kg·m^{-3}	N_p	±	RD[a]
					Dodecane (Continued)					
91-tan/hos	298.15	348.15	19.5	150.8	0.288	0.038	0.163	18	12	o
					Tridecane					
64-doo	303.15	473.15	5.0	500.0	0.630	0.080	0.112	50	16	(o)
					Tetradecane					
70-sny/win	298.15	358.15	0.9	366.8	0.297	0.037	−0.045	113	−5	o
78-gou	298.15	358.15	5.1	40.1	0.354	0.047	0.151	60	12	e
85-tak/ter	298.15	298.15	50.0	50.0	0.102	0.013	−0.102	1	−1	o
87-hol/goe-1	293.15	293.15	2.0	10.0	0.011	0.001	0.004	5	1	o
					Pentadecane					
58-cut/mcm	310.95	408.15	34.5	654.6	0.389	0.048	0.010	63	−9	o
					Hexadecane					
60-boe	393.15	393.15	9.9	117.8	0.411	0.055	0.067	12	2	o
70-sny/win	338.15	358.15	0.4	290.2	0.378	0.048	−0.095	53	−7	o
78-gou					0.813	0.108	0.490	75	35	e
79-dym/you	298.15	373.15	12.0	450.5	0.614	0.077	0.414	23	13	o
85-gla/pet					1.727	0.229	−1.539	63	−57	e
87-hol/goe	293.15	293.15	2.0	10.0	0.023	0.003	−0.022	5	−5	o
87-hol/goe-1	293.15	293.15	2.0	10.0	0.021	0.003	−0.019	5	−5	o
87-mat/rod					1.081	0.145	−0.956	4	−4	e
91-ban/gar	318.15	373.15	1.0	10.0	0.144	0.019	−0.036	60	−12	o
91-tan/hos	298.15	348.15	9.9	150.5	0.525	0.067	0.368	13	9	o

o and (o), from the same source as the compressed liquid density data, available for a part of the temperature range only, respectively; e, from the smoothing equation given in ref 93-cib.

Table 4. Comparison of Relative Densities, $\rho_{rel} = \rho(T,P)/\rho(T,P_{ref})$ (See Eq 1), Calculated from the Fits in Table 2 with the Generalized Representation of *n*-Alkane Densities by Assael et al. [94-ass/dym]

n-alkane	*T* range[a]/K	P_{max}[a]/MPa	RMSD$_r$/%	bias$_r$[b]/%	max dev[b]/%
pentane	278−323	170	0.072	0.037	0.202
hexane	233−333	300	0.123	0.035	0.336
heptane	198−393	205	0.107	0.029	0.389
octane	258−393	320	0.122	−0.008	0.312
nonane	303−423	160	0.117	0.035	0.437
decane	298−348	500	0.103	−0.101	−0.150
undecane	303−373	305	0.175	−0.028	0.429
dodecane	298−393	420	0.144	0.011	0.358
tridecane	303−373	305	0.082	0.046	0.230
tetradecane	298−358	370	0.063	−0.005	0.155
pentadecane[c]	310−410	650	0.431	−0.427	−0.554
hexadecane	298−373	300	0.063	−0.037	−0.109

The temperature and pressure ranges are those of experimental data used for the evaluation of the generalized representation by Assael et al. The density values used in a comparison were generated in 5 K and P_{max}/10 increments. [b] $\{\rho_{rel}$(Table 2) − ρ_{rel}[94-ass/dym]$\}$ 100/ρ_{rel}[94-ass/dym]. [c] T,P_{max} ranges from Table 3, since no data for pentadecane were used by Assael et al. [94-ass/dym] for evaluation of the generalized representation.

tioned alkanes prompt us to the regions where new experimental data are highly desirable.

The examination of the shape of the $B(T,\vec{b})$ curves was not performed for 1-alkanols [94-cib/zik]. Additional tests showed that there are no minima nor inflection points for all fits for 1-alkanols from methanol through 1-decanol except for 1-nonanol (inflection points around 345 K and 370 K were found for the fits I and II, respectively, given by Cibulka and Ziková [94-cib/zik]).

Recently, Assael et al. [94-ass/dym] have developed generalized formulas for the parameters C and B of the Tait equation to calculate the densities of compressed liquid *n*-alkanes. The temperature and pressure ranges of experimental data used to evaluate their generalized representation were rather limited compared to the present correlations; however, the agreement in these ranges is, except for pentadecane, very good, as is illustrated in Table 4 where the values of relative density, $\rho_{rel} = \rho(T,P)/\rho(T,P_{ref})$, are compared to eliminate the effect of the reference line, $\rho(T,P_{ref})$. The deviations $\{\rho_{rel}$(Table 2) − ρ_{rel}[94-ass/dym]$\}$/ρ_{rel}[94-ass/dym] are either within or close to the experimental error and are mostly negative at lower temperatures and pressures and positive at high pressures. This indicates an excellent performance of the generalized representation proposed by Assael et al. Experimental densities of pentadecane (the only data available in our database were those by Cutler et al. [58-cut/mcm]; see Tables 1 and 3), which were not used by Assael et al., show large negative deviations. Since the original values for the reference line, $\rho(T,P_{ref})$, were used for the fit (see Table 3), the deviations cannot be caused by an inconsistency of the $\rho(T,P_{ref})$ values with the reference line from Cibulka [93-cib]. The values reported for dodecane by the same authors [58-cut/mcm] were rejected (see Table 3) due to large (mostly negative) deviations from most of the other published data. Thus it may be concluded that (i) the densities calculated for pentadecane from the generalized equations given by Assael et al. [94-ass/dym] are likely to be closer to the correct ones than the available experimental values and (ii) the fit given for pentadecane in Table 2 should be regarded as a smoothed representation of probably erroneous data measured by Cutler et al. [58-cut/mcm].

Acknowledgment

A part of this work was done during the stay of I.C. in the laboratory of Prof. I. Nagata, Department of Chemical

Engineering, Kanazawa University, Japan; computer and other facilities provided are acknowledged.

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Received for review February 12, 1996. Accepted April 28, 1996.[⊗] Support from the Grant Agency of the Czech Republic within the Grant No. 203/94/0312 is acknowledged.

JE960058M

[⊗] Abstract published in *Advance ACS Abstracts,* June 1, 1996.