# Reviews

## *P*-ρ-*T* Data of Liquids: Summarization and Evaluation. 6. Nonaromatic Hydrocarbons ($C_n$, $n \geq 5$) except *n*-Alkanes $C_5$ to $C_{16}$

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The published experimental data for 56 hydrocarbons (22 alkanes, 11 alkenes, 20 cycloalkanes, and 3 cycloalkenes) are summarized and reviewed, and the parameters of the Tait equation are given. This equation allows the calculation of smoothed values of either the volume ratio $V(P)/V(P_{ref})$ and related properties (relative density $\rho(P)/\rho(P_{ref})$ and compression $\{1 - \rho(P_{ref})/\rho(P)\}$) or, using density data at atmospheric pressure ($P_{ref} = 0.1$ MPa) or at saturation ($P_{ref} = P_{sat}$), the liquid density of the substances over a temperature and pressure range. A comparison of isothermal compressibilities calculated from the Tait equation with available data at $P = 0.1$ MPa from the literature is also presented.

### Introduction

This work is the last part of a systematic summarization and critical evaluation of published $P-\rho-T$ data of hydrocarbons $C_n$, $n \geq 5$, in a liquid state. The data for *n*-alkanes from $C_5$ to $C_{16}$ [96-cib/hne] and aromatic hydrocarbons [99-cib/tak] have already been reviewed and evaluated. This work concerns the remaining groups of hydrocarbons for which the available published experimental values of density, $\rho(T,P)$ relative density $\rho(T,P)/\rho(T,P = 0.1$ MPa or $P_{sat})$, and related quantities of liquids were compiled from the literature and evaluated. The present work and previous reviews [96-cib/hne, 99-cib/tak] do not include compilation or data evaluation for hydrocarbons with less than five carbon atoms; comprehensive reviews of thermodynamic properties (including $P-\rho-T$ surface of the fluid state) for most of these hydrocarbons may be found in the literature [75-zor/hen, 81-bue/mau, 83-wax/gal, 86-jah/jac, 87-you/ely, 89-fri/ely, 91-fri/ing, 91-set/wag].

### Sources of Data

The original experimental data (9576 data points for 56 substances) processed were extracted from the source database which was employed for our previous reviews and is currently being updated. A list of substances is presented in Table 1 along with Chemical Abstracts Service Registry Numbers (CASRN) and formulas.

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 selected compounds are summarized in Table 2. The temperature ranges and numbers of experimental values are restricted up to the critical temperature; that is, only subcritical liquid density data were taken from the source database. No corrections for the different temperature scales were made; the effect is mostly less than the uncertainties in density and/or temperature measurements. Very few researchers declare a particular temperature scale used (see "data type" column and footnotes f through i in Table 2). Similarly, as in our previous reviews, values (denoted by the letter F in the "data type" column of Table 2) calculated from smoothing functions presented in the papers (mostly the Tait equation), following as much as possible the information concerning the distribution of experimental points given by authors, were included for some substances if no direct experimental (D) or smoothed values (S) were available in the papers. The $\rho(T,P)$ values calculated from other properties (C) were also included in the evaluation.

### Treatment of Data and Method of Data Evaluation

The procedures of treatment of the data and the critical evaluation were essentially the same as those employed in our previous papers [96-cib/hne, 99-cib/tak]. A brief summarization only is given below.

Available data on the compressed liquid density and related quantities were fitted by a Tait equation with the temperature-dependent parameters $C(T)$ and $B(T)$, written in the form

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

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**Table 1. List of Substances: Names (Alternative Names), Chemical Abstracts Service Registry Numbers (CASRN, supplied by authors), and Summary Formulas**

| name (alternative name) | CASRN | formula | name (alternative name) | CASRN | formula |
|---|---|---|---|---|---|
| | | | Alkanes | | |
| 2-methylbutane (isopentane) | 78-78-4 | $C_5H_{12}$ | octadecane | 593-45-3 | $C_{18}H_{38}$ |
| 2,2-dimethylpropane (neopentane) | 463-82-1 | $C_5H_{12}$ | 7-hexyltridecane | 7225-66-3 | $C_{19}H_{40}$ |
| 2-methylpentane | 107-83-5 | $C_6H_{14}$ | eicosane | 112-95-8 | $C_{20}H_{42}$ |
| 3-methylpentane | 96-14-0 | $C_6H_{14}$ | docosane | 629-97-0 | $C_{22}H_{46}$ |
| 2,2-dimethylbutane | 75-83-2 | $C_6H_{14}$ | tetracosane | 646-31-1 | $C_{24}H_{50}$ |
| 2,3-dimethylbutane | 79-29-8 | $C_6H_{14}$ | 9-octylheptadecane | 7225-64-1 | $C_{25}H_{52}$ |
| 3-ethylpentane | 617-78-7 | $C_7H_{16}$ | triacontane | 638-68-6 | $C_{30}H_{62}$ |
| 2,2-dimethylpentane | 590-35-2 | $C_7H_{16}$ | 2,6,10,15,19,23-hexamethyltetracosane (squalane) | 111-01-3 | $C_{30}H_{62}$ |
| 2,2,3-trimethylbutane | 464-06-2 | $C_7H_{16}$ | 11-decylheneicosane | 55320-06-4 | $C_{31}H_{64}$ |
| 2,2,4-trimethylpentane (isooctane) | 540-84-1 | $C_8H_{18}$ | 13-dodecylhexacosane | 55517-73-2 | $C_{38}H_{78}$ |
| heptadecane | 629-78-7 | $C_{17}H_{36}$ | tetracontane | 4181-95-7 | $C_{40}H_{82}$ |
| | | | Alkenes | | |
| 2-methyl-1,3-butadiene (isoprene) | 78-79-5 | $C_5H_8$ | 1-hexene | 592-41-6 | $C_6H_{12}$ |
| 1-pentene | 109-67-1 | $C_5H_{10}$ | 1-heptene | 592-76-7 | $C_7H_{14}$ |
| 2-methyl-2-butene (amylene) | 513-35-9 | $C_5H_{10}$ | 1-octene (caprylene) | 111-66-0 | $C_8H_{16}$ |
| (*E*)-1,4-hexadiene | 7319-00-8 | $C_6H_{10}$ | 1-nonene | 124-11-8 | $C_9H_{18}$ |
| (2*Z*,4*E*)-2,4-hexadiene (2-*cis*-4-*trans*-hexadiene) | 5194-50-3 | $C_6H_{10}$ | 2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene (squalene) | 7683-64-9 | $C_{30}H_{50}$ |
| 1,5-hexadiene | 592-42-7 | $C_6H_{10}$ | | | |
| | | | Cycloalkanes | | |
| cyclopentane | 287-92-3 | $C_5H_{10}$ | butylcyclohexane | 1678-93-9 | $C_{10}H_{20}$ |
| methylcyclopentane | 96-37-7 | $C_6H_{12}$ | bicyclohexyl | 92-51-3 | $C_{12}H_{22}$ |
| cyclohexane | 110-82-7 | $C_6H_{12}$ | octadecahydrochrysene (perhydrochrysene) | 2090-14-4 | $C_{18}H_{30}$ |
| cyclohexane-$d_{12}$ (dodecadeuteriocyclohexane) | 1735-17-7 | $C_6D_{12}$ | 1,7-dicyclopentyl-4-(3-cyclopentylpropyl)heptane | 55429-35-1 | $C_{25}H_{46}$ |
| methylcyclohexane | 108-87-2 | $C_7H_{14}$ | 1-(1-decahydronaphthyl)pentadecane | 66359-82-8 | $C_{25}H_{48}$ |
| cycloheptane | 291-64-5 | $C_7H_{14}$ | 1-cyclopentyl-4-(3-cyclopentylpropyl)dodecane | 7225-68-5 | $C_{25}H_{48}$ |
| ethylcyclohexane | 1678-91-7 | $C_8H_{16}$ | 1-cyclohexyl-3-(2-cyclohexylethyl)undecane | 7225-69-6 | $C_{25}H_{48}$ |
| 1-*cis*-2-dimethylcyclohexane | 2207-01-4 | $C_8H_{16}$ | 9-(2-cyclohexylethyl)heptadecane | 25446-35-9 | $C_{25}H_{50}$ |
| cyclooctane | 292-64-8 | $C_8H_{16}$ | 9-(3-cyclopentylpropyl)heptadecane | 5638-09-5 | $C_{25}H_{50}$ |
| *trans*-bicyclo[4.4.0]decane (*trans*-decalin) | 493-02-7 | $C_{10}H_{18}$ | 1,1-bis(decahydro-1-naphthyl)undecane | 55373-96-1 | $C_{31}H_{56}$ |
| | | | Cycloalkenes | | |
| 1,3-cyclohexadiene | 592-57-4 | $C_6H_8$ | cyclohexene | 110-83-8 | $C_6H_{10}$ |
| 1,4-cyclohexadiene | 628-41-1 | $C_6H_8$ | | | |

where

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

$$\vec{c} = \{c_i\} = \{c_0, ..., c_{N_C}\} \quad (2)$$

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

$$\vec{b} = \{b_i\} = \{b_0, ..., b_{N_B}\} \quad (3)$$

and $T_0$ is a parameter with a preselected fixed value for which $C(T_0) = c_0$ and $B(T_0) = b_0$ are valid. The reference values $\rho(T,P_{ref}(T))$ and $P_{ref}(T)$ were selected in the same way as that used previously; that is, at temperatures below the normal boiling temperature, the densities at atmospheric pressure ($P_{ref} = 0.101\ 325$ MPa) were used, while for higher temperatures the values along the saturation curve, that is, saturated liquid densities and saturated vapor pressures, were employed. Experimental values of densities at atmospheric pressure or at saturation for the same sample reported along with compressed liquid density data were preferably used for the reference density $\rho(T,P_{ref})$, and thus the values of relative density $\rho(T,P)/\rho(T,P_{ref} = 0.1$ MPa or $P_{sat})$ reported by the authors were correlated by eq 1. In some cases of isothermal data, the reference density $\rho(T,P_{ref})$ was obtained for each isotherm by an extrapolation of experimental compressed liquid density data to the reference pressure $P_{ref}$ (0.101 325 MPa below or $P_{sat}$ above the normal boiling temperature), using the Tait equation. If the reference values were not available in the original source, and the extrapolation was not feasible (e.g., for isobaric or isochoric data), then the densities obtained from the equations summarized in the Appendix (Table 6) were employed in the correlations. Saturated vapor pressures were calculated from the smoothing functions taken from the literature (for references, see Table 3) and used in the correlations.

The 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 $\rho_j$, $T_j$, $P_j$ is the $j$th experimental data point, $\rho(T_j,P_j,\vec{c},\vec{b})$ is the value calculated from function 1 with the 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 used in the correlation. The adjustable parameters were calculated by the Marquardt algorithm in double precision to minimize the influence of rounding errors. The statistical weights $w_j$ in eq 4 were 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. The uncertainties $\delta\rho_j$ included not only random but also systematic error estimates (if available) and corresponded to the experimental accuracy rather than the precision of measurements. The statistical weight of each density value was adjusted by varying the parameter $\mu_j$ ($\mu_j = 0$ for rejected values), taking into account

**Table 2. 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 | method[a] | data type[b] | sample purity[c]/% |
|---|---|---|---|---|---|---|---|---|
| | | | | 2-Methylbutane | | | | |
| 31-bri | 29 | 273.15 | 368.15 | 49.1 | 882.7 | vb | D | |
| 54-isa/li | 34 | 373.15 | 448.15 | 1.1 | 21.6 | rl | D | 99.89m%[e] |
| 69-mop | 37 | 223.15 | 298.15 | 10.2 | 202.8 | vb | D | 99.99[e] |
| 71-hou/hey | 15 | 298.15 | 298.15 | 50.0 | 2400.0 | vs | S | |
| 74-hou | 12 | 295.15 | 295.15 | 200.0 | 2400.0 | vs | D | |
| 76-sah/gag | 7 | 293.15 | 293.15 | 1.0 | 7.0 | ce | F | 99.9m[e] |
| 92-wal/bar | 180 | 201.40 | 259.90 | 10.0 | 300.0 | vs | S | 99.5[e] |
| total | 314 | 201.40 | 448.15 | 1.0 | 2400.0 | | | |
| | | | | 2,2-Dimethylpropane | | | | |
| 68-gon/lee | 18 | 310.93 | 410.93 | 0.7 | 55.2 | hp | D | 99.92m[e] |
| 73-daw/sil | 61 | 343.15 | 393.15 | 0.6 | 31.6 | vl | D | >99.9[e] |
| 73-koh/luk | 38 | 298.15 | 298.15 | 0.3 | 6.9 | vl | F | >99[d] |
| 75-luk/dav | 49 | 298.15 | 298.15 | 0.3 | 6.6 | vl | F | >99m[d] |
| total | 166 | 298.15 | 410.93 | 0.3 | 55.2 | | | |
| | | | | 2-Methylpentane | | | | |
| 31-bri | 34 | 273.15 | 368.15 | 49.1 | 1176.9 | vb | D | |
| 40-kel/fel | 37 | 373.15 | 473.15 | 0.6 | 31.6 | pi | D[f] | |
| 76-sah/gag | 14 | 293.15 | 298.15 | 1.0 | 7.0 | ce | F | 99.9m[e] |
| 88-mor/aon | 64 | 298.15 | 313.15 | 1.8 | 135.8 | vl | D | |
| total | 149 | 273.15 | 473.15 | 0.6 | 1176.9 | | | |
| | | | | 3-Methylpentane | | | | |
| 31-bri | 40 | 273.15 | 368.15 | 49.1 | 1176.9 | vb | D | |
| 52-day/fel | 76 | 353.15 | 498.15 | 0.6 | 31.6 | vl | D | 99.80m[e] |
| 76-sah/gag | 14 | 293.15 | 298.15 | 1.0 | 7.0 | ce | F | 99.9m[d] |
| 88-mor/aon | 63 | 298.15 | 313.15 | 2.5 | 145.4 | vl | D | |
| total | 193 | 273.15 | 498.15 | 0.6 | 1176.9 | | | |
| | | | | 2,2-Dimethylbutane | | | | |
| 31-bri | 26 | 273.15 | 368.15 | 49.1 | 980.8 | vb | D | |
| 43-fel/wat | 69 | 373.15 | 473.15 | 1.0 | 30.4 | vl | S[f] | |
| 76-sah/gag | 14 | 293.15 | 298.15 | 1.0 | 7.0 | ce | F | 99.9m[e] |
| 88-mor/aon | 58 | 298.15 | 313.15 | 1.5 | 124.3 | vl | D | |
| 90-pol/wei | 72 | 243.70 | 313.20 | 5.0 | 200.0 | vb | F | 99.0[d] |
| total | 239 | 243.70 | 473.15 | 1.0 | 980.8 | | | |
| | | | | 2,3-Dimethylbutane | | | | |
| 31-bri | 32 | 273.15 | 368.15 | 49.1 | 1078.8 | vb | D | |
| 42-kel/fel | 44 | 373.15 | 498.15 | 0.6 | 31.6 | vl | D[f] | |
| 76-sah/gag | 14 | 293.15 | 298.15 | 1.0 | 7.0 | ce | F | 99.9m[d] |
| 87-hol/goe | 5 | 293.15 | 293.15 | 2.0 | 10.0 | mo | D[g] | >99.6m[e] |
| 88-mor/aon | 61 | 298.15 | 313.15 | 1.6 | 139.3 | vl | D | |
| 90-rie/sch | 365 | 173.20 | 303.20 | 10.0 | 300.0 | vs | S | 99.5[d] |
| 93-bao/cac | 215 | 208.16 | 298.15 | 0.2 | 108.5 | rl | D[h] | 99.2m[e] |
| total | 736 | 173.20 | 498.15 | 0.2 | 1078.8 | | | |
| | | | | 3-Ethylpentane | | | | |
| 70-kus/tas | 20 | 298.15 | 353.15 | 39.2 | 196.1 | vl | D | |
| | | | | 2,2-Dimethylpentane | | | | |
| 76-sah/gag | 14 | 293.15 | 298.15 | 1.0 | 7.0 | ce | F | 99.9m[e] |
| | | | | 2,2,3-Trimethylbutane | | | | |
| 70-kus/tas | 11 | 298.15 | 353.15 | 39.2 | 156.9 | vl | D | |
| | | | | 2,2,4-Trimethylpentane | | | | |
| 32-bri | 30 | 273.15 | 368.15 | 49.0 | 980.7 | vb | D | |
| 43-fel/wat-1 | 72 | 373.15 | 523.15 | 0.5 | 30.4 | vl | S | 99.9m[e] |
| 85-dym/isd | 43 | 298.19 | 372.95 | 25.4 | 539.8 | vb | D[g] | >99m[d] |
| 86-hol/goe | 5 | 293.15 | 293.15 | 2.0 | 10.0 | mo | D[g] | >99.8m[e] |
| 87-led | 70 | 298.15 | 358.15 | 10.0 | 330.0 | vb | S | 99.5[d] |
| 90-mal/woo | 115 | 278.15 | 323.15 | 2.5 | 280.0 | vb | F | 99.8m[d] |
| 90-mal/woo | 46 | 323.15 | 338.15 | 2.5 | 280.0 | vb | F | 99.8m[d] |
| 90-pol/wei | 48 | 273.15 | 348.15 | 5.0 | 200.0 | vb | F | 99.5[d] |
| 91-pap/zia | 9 | 298.15 | 298.15 | 2.0 | 33.8 | mo | D | 99.5[d] |
| 92-naz/gas | 77 | 294.15 | 538.65 | 5.0 | 58.9 | bu | D | >99.98[d] |
| 93-mal/woo | 89 | 313.15 | 353.15 | 2.6 | 374.3 | vb | D | |
| 94-pad/far | 30 | 298.15 | 348.15 | 10.1 | 100.1 | mo/bu | D | 99.8[e] |
| 96-hah/ulc | 5 | 293.15 | 293.15 | 2.0 | 10.0 | mo | D | 99.92m[e] |
| 96-pad/far-1 | 47 | 197.93 | 298.15 | 10.1 | 100.1 | mo/bu | D[h] | 99.7[e] |
| 96-pad/far-1 | 30 | 298.15 | 348.16 | 10.1 | 100.1 | mo/bu | D[h] | 99.7[e] |
| total | 716 | 197.93 | 538.65 | 0.5 | 980.7 | | | |
| | | | | Heptadecane | | | | |
| 64-doo | 60 | 323.15 | 573.15 | 5.0 | 500.0 | vl | S | |
| 87-man/cri | 27 | 298.15 | 338.15 | 2.0 | 10.1 | vl | F | 99m[e] |
| total | 87 | 298.15 | 573.15 | 2.0 | 500.0 | | | |

**Table 2. Continued**

| ref | $N_p$ | $T_{min}$/K | $T_{max}$/K | $P_{min}$/MPa | $P_{max}$/MPa | method[a] | data type[b] | sample purity[c]/% |
|---|---|---|---|---|---|---|---|---|
| | | | | Octadecane | | | | |
| 58-cut/mcm | 48 | 333.15 | 408.15 | 34.5 | 551.3 | vb | D | |
| | | | | 7-Hexyltridecane | | | | |
| 59-low/spe | 38 | 310.93 | 408.15 | 20.0 | 340.0 | vb | S | |
| | | | | Eicosane | | | | |
| 64-doo | 50 | 373.15 | 573.15 | 5.0 | 500.0 | vl | S | |
| | | | | Docosane | | | | |
| 88-pet/spi | 48 | 323.08 | 368.26 | 2.1 | 16.1 | ct | D | >99m[e] |
| | | | | Tetracosane | | | | |
| 87-pet/van | 36 | 333.52 | 371.22 | 2.1 | 12.1 | nd | D | >98m[e] |
| | | | | 9-Octylheptadecane | | | | |
| 58-cut/mcm | 140 | 310.95 | 408.15 | 34.5 | 1033.7 | vb | S | |
| 59-low/spe | 20 | 310.93 | 372.04 | 20.0 | 340.0 | vb | S | |
| total | 160 | 310.93 | 408.15 | 20.0 | 1033.7 | | | |
| | | | | Triacontane | | | | |
| 64-doo | 50 | 373.15 | 573.15 | 5.0 | 500.0 | vl | S | |
| | | | | 2,6,10,15,19,23-Hexamethyltetracosane | | | | |
| 70-kus/tas | 20 | 298.15 | 353.15 | 39.2 | 196.1 | vl | D | |
| | | | | 11-Decylheneicosane | | | | |
| 59-low/spe | 36 | 310.93 | 408.15 | 20.0 | 340.0 | vb | S | |
| | | | | 13-Dodecylhexacosane | | | | |
| 59-low/spe | 34 | 310.93 | 408.15 | 20.0 | 340.0 | vb | S | |
| | | | | Tetracontane | | | | |
| 64-doo | 40 | 423.15 | 573.15 | 5.0 | 500.0 | vl | S | |
| | | | | 2-Methyl-1,3-butadiene | | | | |
| 32-bri | 14 | 273.15 | 273.15 | 49.0 | 1176.8 | vb | D | |
| | | | | 1-Pentene | | | | |
| 51-day/fel | 50 | 353.15 | 448.15 | 0.6 | 31.6 | vl | D | 99.34m[e] |
| | | | | 2-Methyl-2-butene | | | | |
| 49-bri | 10 | 298.15 | 298.15 | 49.0 | 490.3 | vs | D | |
| | | | | (*E*)-1,4-Hexadiene | | | | |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99m[d] |
| | | | | (2*Z*,4*E*)-2,4-Hexadiene | | | | |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99m[d] |
| | | | | 1,5-Hexadiene | | | | |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99.9m[d] |
| | | | | 1-Hexene | | | | |
| 70-aba/ker | 192 | 283.15 | 503.15 | 4.0 | 68.7 | bu | D | 99.8[e] |
| 72-ker/apa | 431 | 283.15 | 503.15 | 0.8 | 68.7 | bu | D | 99.98[e] |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99.9m[d] |
| 82-gus/gal | 48 | 146.00 | 293.50 | 5.0 | 50.0 | bu | D | |
| total | 681 | 146.00 | 503.15 | 0.8 | 68.7 | | | |
| | | | | 1-Heptene | | | | |
| 81-gus/naz | 78 | 293.15 | 523.15 | 4.0 | 50.0 | bu | D | |
| | | | | 1-Octene | | | | |
| 49-bri | 17 | 298.15 | 298.15 | 49.0 | 3922.7 | vs | D | |
| 72-ker/apa | 361 | 283.15 | 533.15 | 2.6 | 68.7 | bu | D | 99.98[e] |
| 88-dym/mal | 33 | 298.15 | 373.15 | 10.6 | 312.7 | vb | D | 99m[d] |
| 92-naz/gas | 70 | 290.15 | 538.95 | 5.0 | 58.9 | bu | D | >99.98[d] |
| total | 481 | 283.15 | 538.95 | 2.6 | 3922.7 | | | |
| | | | | 1-Nonene | | | | |
| 84-gus/gal | 70 | 198.00 | 523.00 | 10.0 | 50.0 | bu | D | |
| | | | | 2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene | | | | |
| 70-kus/tas | 20 | 298.15 | 353.15 | 39.2 | 196.1 | vl | D | |
| | | | | Cyclopentane | | | | |
| 69-bra/fre | 9 | 303.15 | 303.15 | 50.0 | 450.0 | vb | D | |
| 70-kus/tas | 20 | 298.15 | 353.15 | 39.2 | 196.1 | vl | D | |
| 92-bao/cac | 186 | 192.79 | 298.15 | 0.1 | 104.3 | rl | D[h] | >99.5m[d] |
| total | 215 | 192.79 | 353.15 | 0.1 | 450.0 | | | |
| | | | | Methylcyclopentane | | | | |
| 80-oza/ooy | 41 | 298.20 | 348.20 | 9.9 | 196.2 | vl | D | 99.9 m[e] |
| 87-hol/goe | 5 | 293.15 | 293.15 | 2.0 | 10.0 | mo | D[g] | >99.6m[e] |
| total | 46 | 293.15 | 348.20 | 2.0 | 196.2 | | | |

**Table 2. Continued**

| ref | $N_p$ | $T_{min}$/K | $T_{max}$/K | $P_{min}$/MPa | $P_{max}$/MPa | method[a] | data type[b] | sample purity[c]/% |
|---|---|---|---|---|---|---|---|---|
| | | | | Cyclohexane | | | | |
| 34-rot/nag | 9 | 289.29 | 291.47 | 0.2 | 20.9 | vl | D | |
| 40-sch/hof | 3 | 311.08 | 377.59 | 5.5 | 5.5 | vl | D | |
| 57-rea/sag | 78 | 310.93 | 510.93 | 0.4 | 68.5 | vl | D[i] | >99.8m[e] |
| 59-gol/vag | 89 | 293.65 | 548.15 | 0.3 | 53.5 | bu | D | |
| 59-gol/vag | 80 | 293.15 | 553.15 | 5.1 | 50.7 | bu | S | |
| 62-hol/wha | 50 | 298.16 | 348.15 | 1.0 | 10.0 | vl | F | >99.9[e] |
| 70-kus/tas | 6 | 313.15 | 353.15 | 39.2 | 117.7 | vl | D | |
| 72-gol/ada | 30 | 303.15 | 393.15 | 50.7 | 253.3 | vb | D | |
| 72-ker/apa | 541 | 283.15 | 553.15 | 1.1 | 68.7 | bu | D | 99.98[e] |
| 72-lys | 2 | 297.15 | 297.15 | 179.0 | 421.0 | sw | D | |
| 73-ker/apa | 368 | 293.15 | 553.16 | 1.1 | 68.7 | bu | D | 99.98[e] |
| 73-rog/bur | 10 | 298.15 | 298.15 | 1.0 | 10.0 | ce | F | |
| 74-apa/ker | 101 | 283.15 | 553.15 | 2.1 | 68.7 | bu | D | >99.98[e] |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | |
| 75-gri/mur | 40 | 498.15 | 548.15 | 2.1 | 79.1 | pi | D | 99.90[e] |
| 75-ras/gri | 96 | 298.15 | 473.15 | 0.6 | 85.4 | pi | D | 99.90[e] |
| 75-ras/gri | 35 | 298.15 | 473.15 | 1.6 | 71.0 | pi | D | 99.90[e] |
| 78-gou | 75 | 314.15 | 393.15 | 5.1 | 40.1 | vl | D | |
| 79-dic | 18 | 295.00 | 295.00 | 1800.0 | 42600.0 | sw | D | 99[d] |
| 79-isd/dym | 4 | 298.15 | 348.15 | 10.0 | 20.0 | ul | C | >99[e] |
| 79-isd/dym | 2 | 348.15 | 348.15 | 50.0 | 100.0 | vb | D | >99[e] |
| 79-kas/fuk | 32 | 298.15 | 348.15 | 6.9 | 105.3 | vl | D | 99.8v[d] |
| 80-jon/has | 40 | 313.00 | 383.00 | 5.0 | 214.0 | vb | D | |
| 82-wis/wue | 27 | 286.80 | 337.90 | 10.0 | 110.0 | vs | S | 99.9[e] |
| 84-mat/van | 34 | 288.15 | 313.15 | 2.5 | 35.0 | mo | F | |
| 87-sun/kor | 80 | 288.15 | 323.06 | 5.0 | 85.0 | ul | C[g] | >99.5v[d] |
| 88-mor/aon | 27 | 298.15 | 313.15 | 2.4 | 46.1 | vl | D | |
| 89-vos/slo | 24 | 326.50 | 450.00 | 0.4 | 10.4 | vs | D | |
| 90-pol/wei | 35 | 293.20 | 368.10 | 5.0 | 180.0 | vb | F | 99.9[d] |
| 90-tos/fig | 48 | 308.07 | 343.15 | 4.6 | 101.9 | bu | D | 99.5m[d] |
| 90-tos/fig | 6 | 333.15 | 333.15 | 39.8 | 91.7 | bu | D | 99.5m[d] |
| 91-mel/mel | 49 | 293.15 | 413.15 | 10.0 | 250.0 | pi | D | |
| 91-tan/hos | 23 | 298.15 | 348.15 | 6.2 | 100.0 | va | D | 99.8[e] |
| 92-lag/bon | 18 | 288.15 | 323.15 | 5.0 | 15.0 | mo[j] | D | |
| 92-lag/bon | 18 | 288.15 | 323.15 | 5.0 | 15.0 | mo[j] | D | |
| 96-pad/far | 20 | 298.15 | 348.14 | 5.1 | 62.8 | mo/bu | D | 99.85[e] |
| total | 2128 | 283.15 | 553.16 | 0.2 | 42600.0 | | | |
| | | | | Cyclohexane-$d_{12}$ | | | | |
| 84-mat/van | 35 | 288.15 | 313.15 | 2.5 | 35.0 | mo | F | |
| | | | | Methylcyclohexane | | | | |
| 49-bri | 11 | 298.15 | 298.15 | 49.0 | 980.7 | vs | D | |
| 69-bra/fre | 9 | 303.15 | 303.15 | 50.0 | 450.0 | vb | D | |
| 70-aba/ker | 255 | 283.15 | 568.15 | 5.0 | 68.7 | bu | D | 99.9[e] |
| 72-ker/apa | 459 | 283.15 | 568.15 | 5.0 | 68.7 | bu | D | 99.98[e] |
| 72-ker/apa | 38 | 283.15 | 568.15 | 0.3 | 6.0 | bu | D | 99.98[e] |
| 78-gou | 90 | 293.15 | 392.55 | 5.1 | 40.1 | vl | D | |
| 79-jon/has | 27 | 203.00 | 298.00 | 50.0 | 500.0 | nd | D | |
| 97-bay/bon | 15 | 303.15 | 343.15 | 20.0 | 100.0 | mo | D | >99[d] |
| total | 904 | 203.00 | 568.15 | 0.3 | 980.7 | | | |
| | | | | Cycloheptane | | | | |
| 70-kus/tas | 12 | 298.15 | 353.15 | 39.2 | 196.1 | vl | D | |
| 78-gou | 90 | 293.65 | 393.15 | 5.1 | 40.1 | vl | D | |
| total | 102 | 293.65 | 393.15 | 5.1 | 196.1 | | | |
| | | | | Ethylcyclohexane | | | | |
| 83-gus/sha | 78 | 293.15 | 523.15 | 5.0 | 50.0 | bu | D | |
| 89-vos/slo | 24 | 327.10 | 440.90 | 0.4 | 9.7 | vs | D | |
| total | 102 | 293.15 | 523.15 | 0.4 | 50.0 | | | |
| | | | | 1-*cis*-2-Dimethylcyclohexane | | | | |
| 89-vos/slo | 21 | 325.20 | 461.20 | 0.4 | 9.7 | vs | D | |
| | | | | Cyclooctane | | | | |
| 78-gou | 75 | 313.65 | 393.85 | 5.1 | 40.1 | vl | D | |
| | | | | *trans*-Bicyclo[4.4.0]decane (*trans*-decalin) | | | | |
| 70-kus/tas | 20 | 298.15 | 353.15 | 39.2 | 196.1 | vl | D | |
| | | | | Butylcyclohexane | | | | |
| 87-hol/goe | 5 | 293.15 | 293.15 | 2.0 | 10.0 | mo | D[g] | >99.8m[e] |
| | | | | Bicyclohexyl | | | | |
| 88-sid/tej | 21 | 298.20 | 338.20 | 0.7 | 34.5 | mo | D | >99m[d] |

**Table 2. Continued**

| ref | $N_p$ | $T_{min}$/K | $T_{max}$/K | $P_{min}$/MPa | $P_{max}$/MPa | method[a] | data type[b] | sample purity[c]/% |
|---|---|---|---|---|---|---|---|---|
| | | | | Octadecahydrochrysene | | | | |
| 59-low/spe | 48 | 310.93 | 408.15 | 20.0 | 340.0 | vb | S | |
| | | | | 1,7-Dicyclopentyl-4-(3-cyclopentylpropyl)heptane | | | | |
| 58-cut/mcm | 113 | 310.95 | 408.15 | 34.5 | 1033.7 | vb | S | |
| | | | | 1-(1-Decahydronaphthyl)pentadecane | | | | |
| 58-cut/mcm | 49 | 333.15 | 408.15 | 34.5 | 585.7 | vb | S | |
| | | | | 1-Cyclopentyl-4-(3-cyclopentylpropyl)dodecane | | | | |
| 58-cut/mcm | 149 | 310.95 | 408.15 | 34.5 | 1033.7 | vb | S | |
| | | | | 1-Cyclohexyl-3-(2-cyclohexylethyl)undecane | | | | |
| 58-cut/mcm | 103 | 310.95 | 408.15 | 34.5 | 895.8 | vb | S | |
| | | | | 9-(2-Cyclohexylethyl)heptadecane | | | | |
| 58-cut/mcm | 126 | 310.95 | 408.15 | 34.5 | 1033.7 | vb | S | |
| | | | | 9-(3-Cyclopentylpropyl)heptadecane | | | | |
| 58-cut/mcm | 139 | 310.95 | 408.15 | 34.5 | 1033.7 | vb | S | |
| | | | | 1,1-Bis(decahydro-1-naphthyl)undecane | | | | |
| 59-low/spe | 35 | 310.93 | 408.15 | 20.0 | 300.0 | vb | S | |
| | | | | 1,3-Cyclohexadiene | | | | |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99m[d] |
| 79-dic | 11 | 295.00 | 295.00 | 920.0 | 41100.0 | sw | D | 97[d] |
| total | 21 | 293.15 | 298.15 | 1.0 | 41100.0 | | | |
| | | | | 1,4-Cyclohexadiene | | | | |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99.7m[d] |
| 79-dic | 11 | 295.00 | 295.00 | 950.0 | 41700.0 | sw | D | 97[d] |
| total | 21 | 293.15 | 298.15 | 1.0 | 41700.0 | | | |
| | | | | Cyclohexene | | | | |
| 72-ker/apa | 364 | 283.15 | 533.15 | 2.6 | 68.7 | bu | D | 99.98[e] |
| 75-bur/ric | 10 | 293.15 | 298.15 | 1.0 | 5.0 | ce | F | 99.9m[d] |
| 79-dic | 15 | 295.00 | 295.00 | 500.0 | 40300.0 | sw | D | 99[d] |
| 91-mel/mel | 70 | 293.15 | 413.15 | 10.0 | 250.0 | pi | D | |
| total | 459 | 283.15 | 533.15 | 1.0 | 40300.0 | | | |

[a] Method used for measurements: bu, buoyancy method; ca, densities obtained by integration from thermal expansivities measured by calorimetric method; ce, densities evaluated by integration from isothermal compressibilities obtained by ultracentrifuge method; ct, Cailletet apparatus; hp, high-pressure pycnometer; mo, mechanical oscillator method; mo/bu, combination of vibrating-wire technique with buoyancy principle; nd, not described or stated in the reference; pi, piezometer of unspecified type; rl, expansion principle; sw, shock wave method; ul, densities evaluated from speeds of ultrasound; va, Aime method; vb, variable-volume cell with bellows; vl, variable-volume cell with liquid piston; vs, variable-volume cell with solid piston. For the classification and description of the methods, see ref [85-tek/cib]. [b] D, direct experimental data; S, smoothed data presented in the reference; C, calculated from other properties; F, values calculated from smoothing equation reported by the researchers. [c] No letter, unspecified percent; m, mole percent; v, volume 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] IPTS-68 declared by the researchers. [h] ITS-90 declared by the researchers. [i] ITS-48 declared by the researchers. [j] Two methods of calibration of DMA 512 vibrating-tube densimeter reported; the first one declared to be superior.

additional available information (sample purity, experimental method used, uncertainties in temperature and pressure measurements). In some cases comparisons of isothermal compressibilities calculated from the fit of a particular data set with independent values (see below and Table 5) were made to facilitate the adjustment. The calculations of the parameters $\vec{c}$ and $\vec{b}$ were repeated until the final fit was obtained where the deviations between retained experimental and smoothed values were roughly equal to the modified experimental uncertainties, $\delta\rho_j/\mu_j^{1/2}$, that is, where the weighted standard deviation of the fit was close to unity. In those cases where only one set of smoothed values (S-type data, Table 2) was available for a particular substance, the statistical weights were not modified ($\mu_j = 1$ for retained and $\mu_j = 0$ for rejected data points) and therefore the weighted standard deviation $s_w$ (see below) may differ from unity.

## Results

Table 3 records the values of the parameters of eq 1 for each substance 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. The characteristics are given on an absolute density scale ($kg\cdot m^{-3}$), which is more illustrative than on a relative density scale.

**Table 3. 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 ($N_p$), ±, Weighted Standard Deviations ($s_w$), and References to Saturated Vapor Pressure (ref($P_{sat}$)) for the Fits Where $T_{max}$ Is Higher Than the Normal Boiling Temperature**

| | 2-methyl-butane | 2,2-dimethyl-propane | 2-methyl-pentane | 3-methyl-pentane | 2,2-dimethyl-butane | 2,3-dimethyl-butane | 2,3-dimethyl-butane[b] | 3-ethyl-pentane |
|---|---|---|---|---|---|---|---|---|
| $c_0$ | 0.088008 | 0.086510 | 0.089537 | 0.087915 | 0.088950 | 0.073172 | 0.087435 | 0.091852 |
| $c_1$/K$^{-1}$ | | | | | | 0.004085 | | |
| $b_0$/MPa | 97.8313 | 27.3297 | 49.8393 | 48.9510 | 45.1214 | 39.8600 | 48.8186 | 67.8829 |
| $b_1$/(MPa·K$^{-1}$) | −84.7915 | −34.2103 | −49.6496 | −44.2980 | −43.9956 | −38.8467 | −40.2085 | −57.8087 |
| $b_2$/(MPa·K$^{-2}$) | 23.2045 | 7.6955 | 14.4427 | 9.2935 | 10.1425 | 11.2092 | −30.9644 | 19.1434 |
| $b_3$/(MPa·K$^{-3}$) | | | −1.3079 | | | −1.2447 | | |
| $T_0$/K | 201.40 | 298.15 | 298.15 | 303.15 | 298.15 | 298.15 | 298.15 | 298.15 |
| $T_{min}$/K | 223.15 | 298.15 | 273.15 | 293.15 | 243.70 | 208.16 | 293.15 | 298.15 |
| $T_{max}$/K | 298.15 | 393.15 | 473.15 | 473.15 | 473.15 | 473.15 | 313.15 | 353.15 |
| $P_{min}$/MPa | 1.00 | 0.30 | 0.57 | 0.57 | 1.00 | 0.18 | 1.00 | 39.23 |
| $P_{max}$/MPa | 2400.00 | 31.58 | 1176.90 | 145.40 | 200.00 | 106.25 | 139.30 | 196.13 |
| RMSD/(kg·m$^{-3}$) | 0.440 | 0.207 | 2.199 | 0.453 | 0.496 | 0.477 | 0.189 | 0.128 |
| RMSD$_r$/% | 0.057 | 0.041 | 0.272 | 0.086 | 0.089 | 0.072 | 0.027 | 0.017 |
| bias/(kg·m$^{-3}$) | −0.115 | 0.041 | −0.042 | 0.040 | −0.016 | −0.165 | −0.049 | 0.000 |
| $N_p$ | 56 | 148 | 141 | 140 | 210 | 280 | 80 | 20 |
| ± | −10 | −2 | 11 | −8 | 20 | −104 | −20 | 0 |
| $s_w$ | 0.914 | 1.092 | 1.140 | 1.140 | 1.095 | 1.214 | 1.057 | 1.012 |
| ref($P_{sat}$) | | 83-mcg | 83-mcg | 83-mcg | 83-mcg | 83-mcg | | |

| | 2,2-dimethyl-pentane | 2,2,3-trimethyl-butane | 2,2,4-trimethyl-pentane | heptadecane | octadecane | 7-hexyltridecane | eicosane | docosane |
|---|---|---|---|---|---|---|---|---|
| $c_0$ | 0.079479 | 0.090175 | 0.087786 | 0.087728 | 0.087801 | 0.088830 | 0.086743 | 0.039049 |
| $b_0$/MPa | 50.5418 | 37.2254 | 46.4381 | 89.5233 | 56.3108 | 68.8356 | 68.2027 | 38.0546 |
| $b_1$/(MPa·K$^{-1}$) | −59.0336 | −29.6553 | −39.8361 | −53.2648 | −34.8999 | −44.6628 | −43.1426 | −43.4898 |
| $b_2$/(MPa·K$^{-2}$) | | 23.8796 | 10.6744 | 8.7057 | 14.5622 | 8.8493 | 7.6667 | 39.1505 |
| $b_3$/(MPa·K$^{-3}$) | | | −2.4092 | | | | | |
| $b_4$/(MPa·K$^{-4}$) | | | 0.5894 | | | | | |
| $T_0$/K | 293.15 | 353.15 | 323.15 | 323.15 | 408.15 | 372.04 | 373.15 | 323.08 |
| $T_{min}$/K | 293.15 | 298.15 | 197.93 | 298.15 | 333.15 | 310.93 | 373.15 | 323.08 |
| $T_{max}$/K | 298.15 | 353.15 | 523.15 | 573.15 | 408.15 | 408.15 | 573.15 | 368.26 |
| $P_{min}$/MPa | 1.00 | 39.23 | 0.51 | 2.03 | 34.46 | 20.00 | 5.00 | 2.05 |
| $P_{max}$/MPa | 7.00 | 156.91 | 882.60 | 500.00 | 551.28 | 340.00 | 500.00 | 16.05 |
| RMSD/(kg·m$^{-3}$) | 0.005 | 0.082 | 0.639 | 0.944 | 0.403 | 0.230 | 1.222 | 0.422 |
| RMSD$_r$/% | 0.001 | 0.011 | 0.091 | 0.121 | 0.051 | 0.028 | 0.159 | 0.055 |
| bias/(kg·m$^{-3}$) | 0.001 | −0.001 | −0.082 | 0.035 | 0.023 | 0.027 | 0.067 | −0.001 |
| $N_p$ | 14 | 11 | 446 | 87 | 48 | 36 | 50 | 48 |
| ± | 2 | 1 | −56 | −11 | −4 | −2 | 0 | −16 |
| $s_w$ | 0.007 | 0.920 | 1.124 | 0.853 | 0.907 | 0.899 | 0.797 | 1.138 |
| ref($P_{sat}$) | | | 83-mcg | | | | | |

| | tetracosane | 9-octyl-heptadecane | triacontane | HMTC[c] | 11-decyl-heneicosane | 13-dodecyl-hexacosane | tetracontane | 2-methyl-1,3-butadiene |
|---|---|---|---|---|---|---|---|---|
| $c_0$ | 0.057048 | 0.092203 | 0.086183 | 0.090208 | 0.088556 | 0.089487 | 0.086751 | 0.099097 |
| $b_0$/MPa | 54.7838 | 84.8571 | 81.9415 | 122.1435 | 84.9378 | 90.1315 | 66.5183 | 80.8813 |
| $b_1$/(MPa·K$^{-1}$) | −31.0645 | −48.6706 | −53.8673 | −52.1931 | −46.0832 | −46.9989 | −41.3867 | |
| $b_2$/(MPa·K$^{-2}$) | | 12.2404 | 15.3258 | −4.5813 | 6.0890 | 8.1517 | 9.0745 | |
| $b_3$/(MPa·K$^{-3}$) | | | −2.0531 | | | | | |
| $T_0$/K | 333.52 | 372.05 | 373.15 | 298.15 | 372.04 | 372.04 | 423.15 | 273.15 |
| $T_{min}$/K | 333.52 | 310.93 | 373.15 | 298.15 | 310.93 | 310.93 | 423.15 | 273.15 |
| $T_{max}$/K | 371.22 | 408.15 | 573.15 | 353.15 | 408.15 | 408.15 | 573.15 | 273.15 |
| $P_{min}$/MPa | 2.07 | 20.00 | 5.00 | 39.23 | 40.00 | 20.00 | 5.00 | 49.03 |
| $P_{max}$/MPa | 12.07 | 1033.65 | 500.00 | 196.13 | 340.00 | 340.00 | 500.00 | 1176.80 |
| RMSD/(kg·m$^{-3}$) | 0.195 | 0.655 | 0.973 | 0.057 | 0.302 | 0.226 | 1.267 | 0.568 |
| RMSD$_r$/% | 0.026 | 0.075 | 0.124 | 0.007 | 0.036 | 0.027 | 0.159 | 0.064 |
| bias/(kg·m$^{-3}$) | 0.000 | 0.060 | 0.099 | 0.000 | 0.022 | 0.029 | 0.142 | 0.041 |
| $N_p$ | 36 | 136 | 47 | 20 | 31 | 30 | 40 | 14 |
| ± | −12 | 4 | 11 | 0 | 1 | 4 | 8 | 2 |
| $s_w$ | 0.258 | 0.910 | 0.621 | 0.284 | 0.260 | 0.193 | 0.799 | 0.906 |

| | 1-pentene | 2-methyl-2-butene | (*E*)-1,4-hexadiene | (2*Z*,4*E*)-2,4-hexadiene | 1,5-hexadiene | 1-hexene | 1-heptene | 1-octene |
|---|---|---|---|---|---|---|---|---|
| $c_0$ | 0.080544 | 0.096076 | 0.076611 | 0.075707 | 0.084083 | 0.085421 | 0.136085 | 0.089528 |
| $b_0$/MPa | 6.2555 | 51.9434 | 51.6052 | 60.1053 | 53.5627 | 51.1564 | 117.6648 | 67.6214 |
| $b_1$/(MPa·K$^{-1}$) | −20.6345 | | −55.3701 | −60.7677 | −54.8755 | −49.5730 | −105.5210 | −39.3409 |
| $b_2$/(MPa·K$^{-2}$) | 9.3081 | | | | | 14.4725 | | 1.7555 |
| $b_3$/(MPa·K$^{-3}$) | | | | | | −1.0687 | | 1.2891 |
| $b_4$/(MPa·K$^{-4}$) | | | | | | −0.2793 | | |
| $T_0$/K | 398.15 | 298.15 | 293.15 | 293.15 | 293.15 | 298.15 | 293.15 | 298.15 |
| $T_{min}$/K | 353.15 | 298.15 | 293.15 | 293.15 | 293.15 | 146.00 | 293.15 | 290.15 |
| $T_{max}$/K | 448.15 | 298.15 | 298.15 | 298.15 | 298.15 | 473.15 | 353.15 | 538.95 |
| $P_{min}$/MPa | 0.57 | 49.03 | 1.00 | 1.00 | 1.00 | 0.81 | 5.00 | 5.00 |
| $P_{max}$/MPa | 31.60 | 490.33 | 5.00 | 5.00 | 5.00 | 68.75 | 50.00 | 312.70 |
| RMSD/(kg·m$^{-3}$) | 0.453 | 0.205 | 0.002 | 0.002 | 0.001 | 1.017 | 1.162 | 1.337 |
| RMSD$_r$/% | 0.090 | 0.027 | 0.000 | 0.000 | 0.000 | 0.159 | 0.169 | 0.205 |
| bias/(kg·m$^{-3}$) | −0.056 | 0.014 | 0.000 | 0.000 | 0.000 | −0.246 | −0.165 | 0.321 |
| $N_p$ | 50 | 10 | 10 | 10 | 10 | 418 | 23 | 100 |
| ± | −20 | −4 | 2 | 2 | −2 | −106 | −7 | 14 |
| $s_w$ | 1.066 | 1.150 | 0.036 | 0.029 | 0.013 | 1.153 | 1.200 | 1.659 |
| ref($P_{sat}$) | 83-mcg | | | | | 83-mcg | | 79-dyk/rep |

**Table 3. Continued**

| | 1-nonene | HMTE[d] | cyclopentane | methyl-cyclopentane | cyclohexane | cyclohexane-$d_{12}$ | methyl-cyclohexane |
|---|---|---|---|---|---|---|---|
| $c_0$ | 0.177574 | 0.091245 | 0.088558 | 0.088019 | 0.085159 | 0.079666 | 0.086999 |
| $b_0$/MPa | 381.1410 | 139.3681 | 67.5860 | 55.0075 | 60.3130 | 70.2463 | 80.3279 |
| $b_1$/(MPa·K$^{-1}$) | −215.6507 | −59.0280 | −61.0179 | −50.0741 | −53.8926 | −65.3112 | −63.5774 |
| $b_2$/(MPa·K$^{-2}$) | 36.9232 | | 17.2997 | −8.2772 | 17.0338 | −39.6447 | 17.2095 |
| $b_3$/(MPa·K$^{-3}$) | | | −5.3135 | | −3.8318 | | −1.9196 |
| $b_4$/(MPa·K$^{-4}$) | | | 4.4400 | | 0.5957 | | |
| $T_0$/K | 198.00 | 298.15 | 298.15 | 323.20 | 323.15 | 298.15 | 293.15 |
| $T_{min}$/K | 198.00 | 298.15 | 192.79 | 293.15 | 286.80 | 288.15 | 203.00 |
| $T_{max}$/K | 398.00 | 353.15 | 353.15 | 348.20 | 523.15 | 313.15 | 523.15 |
| $P_{min}$/MPa | 10.00 | 39.23 | 0.12 | 2.00 | 0.57 | 2.50 | 0.35 |
| $P_{max}$/MPa | 50.00 | 196.13 | 196.13 | 196.20 | 250.00 | 35.00 | 500.00 |
| RMSD/(kg·m$^{-3}$) | 0.694 | 0.098 | 0.405 | 0.484 | 0.654 | 0.022 | 0.418 |
| RMSD$_r$/% | 0.092 | 0.011 | 0.050 | 0.063 | 0.087 | 0.002 | 0.053 |
| bias/(kg·m$^{-3}$) | −0.018 | 0.002 | 0.052 | −0.173 | 0.024 | −0.001 | 0.020 |
| $N_p$ | 44 | 20 | 200 | 46 | 708 | 35 | 122 |
| ± | 0 | 4 | 22 | −12 | −46 | −3 | 16 |
| $s_w$ | 0.923 | 0.982 | 0.862 | 0.841 | 0.966 | 0.945 | 0.905 |
| ref($P_{sat}$) | | | 83-mcg | 83-mcg | 83-mcg | | 83-mcg |

| | cycloheptane | ethylcyclohexane | 1-*cis*-2-dimethylcyclooctane | cyclooctane | *trans*-bicyclo[4.4.0]decane | butylcyclohexane |
|---|---|---|---|---|---|---|
| $c_0$ | 0.090935 | 0.110464 | 0.217447 | 0.086604 | 0.092138 | 0.100791 |
| $b_0$/MPa | 103.3619 | 127.7228 | 154.2895 | 98.4214 | 125.1795 | 113.3482 |
| $b_1$/(MPa·K$^{-1}$) | −62.9119 | −116.7650 | −72.7266 | −63.1555 | −56.0076 | |
| $b_2$/(MPa·K$^{-2}$) | 4.2958 | 67.1444 | | 9.0089 | −8.5697 | |
| $b_3$/(MPa·K$^{-3}$) | | −27.1569 | | | | |
| $b_4$/(MPa·K$^{-4}$) | | 4.6173 | | | | |
| $T_0$/K | 293.65 | 293.15 | 325.20 | 313.65 | 298.15 | 293.15 |
| $T_{min}$/K | 293.65 | 293.15 | 325.20 | 313.65 | 298.15 | 293.15 |
| $T_{max}$/K | 393.15 | 523.15 | 461.20 | 393.85 | 353.15 | 293.15 |
| $P_{min}$/MPa | 5.10 | 0.40 | 0.40 | 5.10 | 39.23 | 2.00 |
| $P_{max}$/MPa | 196.13 | 50.00 | 9.70 | 40.10 | 196.13 | 10.00 |
| RMSD/(kg·m$^{-3}$) | 0.330 | 0.842 | 0.625 | 0.211 | 0.019 | 0.003 |
| RMSD$_r$/% | 0.041 | 0.117 | 0.082 | 0.026 | 0.002 | 0.000 |
| bias/(kg·m$^{-3}$) | 0.135 | 0.072 | −0.043 | −0.003 | 0.000 | 0.000 |
| $N_p$ | 102 | 93 | 21 | 75 | 20 | 5 |
| ± | 40 | 9 | −2 | −3 | 2 | 1 |
| $s_w$ | 0.946 | 0.987 | 0.041 | 0.833 | 0.898 | 0.129 |
| ref($P_{sat}$) | | 79-dyk/rep | 83-mcg | 84-bou/fri | | |

| | bicyclohexyl | octadecahydrochrysene | DPPH[e] | 1-(1-decahydronaphthyl)pentadecane | CPPD[f] | CHHU[g] |
|---|---|---|---|---|---|---|
| $c_0$ | 0.132677 | 0.084675 | 0.090467 | 0.087100 | 0.092672 | 0.092218 |
| $b_0$/MPa | 204.0178 | 117.2289 | 88.6294 | 84.8348 | 103.1264 | 88.5456 |
| $b_1$/(MPa·K$^{-1}$) | −89.8586 | −58.9065 | −44.0926 | −46.9197 | −54.0928 | −51.7083 |
| $b_2$/(MPa·K$^{-2}$) | | 7.4154 | 17.6652 | 10.3755 | 14.6027 | 7.6328 |
| $T_0$/K | 298.20 | 388.15 | 408.15 | 408.15 | 372.05 | 408.15 |
| $T_{min}$/K | 298.20 | 310.93 | 310.95 | 333.15 | 310.95 | 310.95 |
| $T_{max}$/K | 338.20 | 408.15 | 408.15 | 408.15 | 408.15 | 408.15 |
| $P_{min}$/MPa | 0.69 | 20.00 | 34.46 | 34.46 | 34.46 | 34.46 |
| $P_{max}$/MPa | 34.48 | 340.00 | 1033.65 | 585.74 | 1033.65 | 895.83 |
| RMSD/(kg·m$^{-3}$) | 0.199 | 0.359 | 0.741 | 0.445 | 1.209 | 0.869 |
| RMSD$_r$/% | 0.023 | 0.036 | 0.077 | 0.049 | 0.128 | 0.093 |
| bias/(kg·m$^{-3}$) | −0.039 | −0.025 | 0.052 | 0.025 | 0.070 | 0.067 |
| $N_p$ | 21 | 48 | 113 | 49 | 149 | 103 |
| ± | −3 | −6 | −11 | 11 | 3 | 11 |
| $s_w$ | 0.993 | 0.257 | 0.553 | 0.352 | 0.914 | 0.664 |

| | 9-(2-cyclohexylethyl)heptadecane | 9-(3-cyclopentylpropyl)heptadecane | DHNU[h] | 1,3-cyclohexadiene | 1,4-cyclohexadiene | cyclohexene |
|---|---|---|---|---|---|---|
| $c_0$ | 0.089788 | 0.092100 | 0.081991 | 0.068186 | 0.088429 | 0.053518 |
| $b_0$/MPa | 74.5186 | 94.3384 | 100.3959 | 69.6306 | 101.2434 | 53.7914 |
| $b_1$/(MPa·K$^{-1}$) | −44.2218 | −51.2070 | −43.0062 | −63.7668 | −127.0709 | −52.3852 |
| $b_2$/(MPa·K$^{-2}$) | 11.8896 | | 21.8428 | | | 16.0062 |
| $T_0$/K | 408.15 | 372.05 | 388.15 | 295.00 | 295.00 | 293.15 |
| $T_{min}$/K | 310.95 | 310.95 | 310.93 | 293.15 | 293.15 | 293.15 |
| $T_{max}$/K | 408.15 | 408.15 | 408.15 | 298.15 | 298.15 | 353.15 |
| $P_{min}$/MPa | 34.46 | 34.46 | 20.00 | 1.00 | 1.00 | 1.00 |
| $P_{max}$/MPa | 1033.65 | 1033.65 | 300.00 | 5.00 | 5.00 | 250.00 |
| RMSD/(kg·m$^{-3}$) | 0.501 | 0.563 | 0.589 | 0.002 | 0.002 | 2.480 |
| RMSD$_r$/% | 0.054 | 0.062 | 0.062 | 0.000 | 0.000 | 0.298 |
| bias/(kg·m$^{-3}$) | 0.028 | 0.048 | 0.094 | 0.000 | 0.000 | −1.117 |
| $N_p$ | 126 | 139 | 35 | 10 | 10 | 50 |
| ± | 0 | −17 | 7 | 0 | 0 | −30 |
| $s_w$ | 0.390 | 0.447 | 0.447 | 0.030 | 0.026 | 1.367 |

[a] The low limit of the 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 correlation. [b] Narrow temperature range fit. [c] HMTC = 2,6,10,15,19,23-hexamethyltetracosane. [d] HMTE = 2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene. [e] DPPH = 1,7-dicyclopentyl-4-(3-cyclopentylpropyl) heptane. [f] CPPD = 1-cyclopentyl-4-(3-cyclopentylpropyl)dodecane. [g] CHHU = 1-cyclohexyl-3-(2-cyclohexylethyl)undecane. [h] DHNU = 1,1-bis(decahydro-1-naphthyl)undecane.

**Table 4. Statistical Characteristics of Individual Data Sets for the Fits in Table 3: 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] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | 2-Methylbutane | | | | | | |
| 31-bri | | | | | 4.819 | 0.579 | 3.560 | 9 | 9 | o |
| 54-isa/li | 0 0 | | | | | | | | | |
| 69-mop | 223.15 | 298.15 | 10.2 | 202.8 | 0.382 | 0.054 | 0.011 | 37 | 1 | o |
| 71-hou/hey | | | | | 5.155 | 0.599 | −4.962 | 15 | −15 | o |
| 74-hou | 295.15 | 295.15 | 200.0 | 2400.0 | 0.675 | 0.077 | −0.571 | 12 | −10 | o |
| 76-sah/gag | 293.15 | 293.15 | 1.0 | 7.0 | 0.015 | 0.002 | −0.002 | 7 | −1 | o |
| 92-wal/bar | | | | | 4.861 | 0.400 | −4.914 | 88 | −86 | o |
| | | | | 2,2-Dimethylpropane | | | | | | |
| 68-gon/lee | | | | | 6.122 | 1.041 | 2.508 | 12 | 6 | p |
| 73-daw/sil | 343.15 | 393.15 | 0.6 | 31.6 | 0.322 | 0.064 | 0.100 | 61 | 25 | p |
| 73-koh/luk | 298.15 | 298.15 | 0.3 | 6.9 | 0.022 | 0.004 | 0.009 | 38 | 6 | o |
| 75-luk/dav | 298.15 | 298.15 | 0.3 | 6.6 | 0.011 | 0.002 | −0.008 | 49 | −33 | o |
| | | | | 2-Methylpentane | | | | | | |
| 31-bri | 273.15 | 368.15 | 196.2 | 1176.9 | 4.994 | 0.587 | −0.174 | 26 | 4 | o |
| 40-kel/fel | 373.15 | 473.15 | 0.6 | 31.6 | 0.912 | 0.198 | −0.015 | 37 | 1 | p |
| 76-sah/gag | 293.15 | 298.15 | 1.0 | 7.0 | 0.041 | 0.006 | 0.031 | 14 | 10 | o |
| 88-mor/aon | 298.15 | 313.15 | 1.8 | 135.8 | 0.189 | 0.028 | −0.020 | 64 | −4 | o |
| | | | | 3-Methylpentane | | | | | | |
| 31-bri | | | | | 5.892 | 0.827 | 5.785 | 5 | 5 | o |
| 52-day/fel | 353.15 | 473.15 | 0.6 | 31.6 | 0.656 | 0.127 | 0.109 | 63 | 11 | p |
| 76-sah/gag | 293.15 | 298.15 | 1.0 | 7.0 | 0.102 | 0.015 | −0.089 | 14 | −14 | o |
| 88-mor/aon | 298.15 | 313.15 | 2.5 | 145.4 | 0.156 | 0.022 | −0.001 | 63 | −5 | o |
| | | | | 2,2-Dimethylbutane | | | | | | |
| 31-bri | | | | | 71.770 | 10.155 | −55.372 | 11 | −11 | o |
| 43-fel/wat | 373.15 | 473.15 | 1.0 | 30.4 | 0.740 | 0.144 | −0.098 | 66 | −16 | p |
| 76-sah/gag | 293.15 | 298.15 | 1.0 | 7.0 | 0.088 | 0.014 | 0.066 | 14 | 12 | o |
| 88-mor/aon | 298.15 | 313.15 | 1.5 | 124.3 | 0.271 | 0.039 | −0.048 | 58 | 0 | o |
| 90-pol/wei | 243.70 | 313.20 | 5.0 | 200.0 | 0.393 | 0.052 | 0.070 | 72 | 24 | o |
| | | | | 2,3-Dimethylbutane | | | | | | |
| 31-bri | | | | | 4.188 | 0.579 | 3.704 | 5 | 5 | o |
| 42-kel/fel | 373.15 | 473.15 | 0.6 | 31.6 | 0.651 | 0.114 | 0.010 | 37 | 1 | o |
| 76-sah/gag | 293.15 | 298.15 | 1.0 | 7.0 | 0.159 | 0.024 | −0.145 | 14 | −14 | o |
| 87-hol/goe | 293.15 | 293.15 | 2.0 | 10.0 | 0.041 | 0.006 | 0.017 | 5 | 1 | o |
| 88-mor/aon | 298.15 | 313.15 | 1.6 | 36.8 | 0.265 | 0.040 | −0.013 | 22 | −4 | o |
| 90-rie/sch | | | | | 4.266 | 0.608 | −0.976 | 140 | −40 | o |
| 93-bao/cac | 208.16 | 298.15 | 0.2 | 106.3 | 0.478 | 0.068 | −0.220 | 202 | −88 | o |
| | | | | 2,3-Dimethylbutane (Narrow Temperature Range Fit) | | | | | | |
| 31-bri | | | | | | | | 0 | 0 | |
| 42-kel/fel | | | | | | | | 0 | 0 | |
| 76-sah/gag | 293.15 | 298.15 | 1.0 | 7.0 | 0.125 | 0.019 | −0.108 | 14 | −14 | o |
| 87-hol/goe | 293.15 | 293.15 | 2.0 | 10.0 | 0.012 | 0.002 | 0.009 | 5 | 3 | o |
| 88-mor/aon | 298.15 | 313.15 | 1.6 | 139.3 | 0.208 | 0.030 | −0.040 | 61 | −9 | o |
| 90-rie/sch | | | | | 4.831 | 0.688 | −4.561 | 26 | −26 | o |
| 93-bao/cac | | | | | 2.481 | 0.349 | −2.047 | 51 | −49 | o |
| | | | | 3-Ethylpentane | | | | | | |
| 70-kus/tas | 298.15 | 353.15 | 39.2 | 196.1 | 0.128 | 0.017 | 0.000 | 20 | 0 | o |
| | | | | 2,2-Dimethylpentane | | | | | | |
| 76-sah/gag | 293.15 | 298.15 | 1.0 | 7.0 | 0.005 | 0.001 | 0.001 | 14 | 2 | o |
| | | | | 2,2,3-Trimethylbutane | | | | | | |
| 70-kus/tas | 298.15 | 353.15 | 39.2 | 156.9 | 0.082 | 0.011 | −0.001 | 11 | 1 | o |
| | | | | 2,2,4-Trimethylpentane | | | | | | |
| 32-bri | 273.15 | 323.15 | 392.3 | 882.6 | 1.290 | 0.145 | 0.471 | 8 | 2 | o |
| 43-fel/wat-1 | 373.15 | 523.15 | 0.5 | 30.4 | 0.714 | 0.134 | 0.218 | 69 | 31 | p |
| 85-dym/isd | 298.19 | 372.95 | 25.4 | 539.8 | 0.552 | 0.070 | 0.139 | 43 | 11 | o |
| 86-hol/goe | 293.15 | 293.15 | 2.0 | 10.0 | 0.014 | 0.002 | 0.010 | 5 | 5 | o |
| 87-led | | | | | 3.426 | 0.438 | 2.884 | 70 | 70 | o |
| 90-mal/woo | 278.15 | 313.15 | 2.5 | 280.0 | 0.236 | 0.031 | −0.112 | 92 | −56 | o |
| 90-mal/woo | | | | | 1.220 | 0.163 | −1.130 | 46 | −46 | o |
| 90-pol/wei | 273.15 | 348.15 | 5.0 | 200.0 | 0.683 | 0.087 | −0.303 | 48 | −14 | o |
| 91-pap/zia | | | | | 0.918 | 0.130 | −0.823 | 9 | −9 | o |
| 92-naz/gas | | | | | 7.699 | 1.313 | −3.564 | 0 | −60 | op |
| 93-mal/woo | 313.15 | 353.15 | 2.6 | 374.3 | 0.584 | 0.076 | −0.160 | 89 | −19 | o |
| 94-pad/far | 298.15 | 348.15 | 10.1 | 100.1 | 0.648 | 0.090 | 0.544 | 30 | 30 | o |
| 96-hah/ulc | 293.15 | 293.15 | 2.0 | 10.0 | 0.018 | 0.003 | −0.010 | 5 | −3 | o |
| 96-pad/far-1 | 197.93 | 248.35 | 10.1 | 100.1 | 1.039 | 0.134 | −0.663 | 27 | −17 | o |
| 96-pad/far-1 | 298.15 | 348.16 | 10.1 | 100.1 | 0.833 | 0.114 | −0.683 | 30 | −26 | o |
| | | | | Heptadecane | | | | | | |
| 64-doo | 323.15 | 573.15 | 5.0 | 500.0 | 1.136 | 0.145 | 0.054 | 60 | −2 | o |
| 87-man/cri | 298.15 | 338.15 | 2.0 | 10.1 | 0.071 | 0.009 | −0.006 | 27 | −9 | o |

**Table 4. 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] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Octadecane | | | | | |
| 58-cut/mcm | 333.15 | 408.15 | 34.5 | 551.3 | 0.403 | 0.051 | 0.023 | 48 | −4 | o |
| | | | | | 7-Hexyltridecane | | | | | |
| 59-low/spe | 310.93 | 408.15 | 20.0 | 340.0 | 0.230 | 0.028 | 0.027 | 36 | −2 | o |
| | | | | | Eicosane | | | | | |
| 64-doo | 373.15 | 573.15 | 5.0 | 500.0 | 1.222 | 0.159 | 0.067 | 50 | 0 | o |
| | | | | | Docosane | | | | | |
| 88-pet/spi | 323.08 | 368.26 | 2.1 | 16.1 | 0.422 | 0.055 | −0.001 | 48 | −16 | p |
| | | | | | Tetracosane | | | | | |
| 87-pet/van | 333.52 | 371.22 | 2.1 | 12.1 | 0.195 | 0.026 | 0.000 | 36 | −12 | p |
| | | | | | 9-Octylheptadecane | | | | | |
| 58-cut/mcm | 310.95 | 408.15 | 34.5 | 1033.7 | 0.640 | 0.072 | −0.051 | 116 | −16 | o |
| 59-low/spe | 310.93 | 372.04 | 20.0 | 340.0 | 0.737 | 0.089 | 0.703 | 20 | 20 | o |
| | | | | | Triacontane | | | | | |
| 64-doo | 373.15 | 573.15 | 5.0 | 500.0 | 0.973 | 0.124 | 0.099 | 47 | 11 | o |
| | | | | | 2,6,10,15,19,23-Hexamethyltetracosane | | | | | |
| 70-kus/tas | 298.15 | 353.15 | 39.2 | 196.1 | 0.057 | 0.007 | 0.000 | 20 | 0 | o |
| | | | | | 11-Decylheneicosane | | | | | |
| 59-low/spe | 310.93 | 408.15 | 40.0 | 340.0 | 0.302 | 0.036 | 0.022 | 31 | 1 | o |
| | | | | | 13-Dodecylhexacosane | | | | | |
| 59-low/spe | 310.93 | 408.15 | 20.0 | 340.0 | 0.226 | 0.027 | 0.029 | 30 | 4 | o |
| | | | | | Tetracontane | | | | | |
| 64-doo | 423.15 | 573.15 | 5.0 | 500.0 | 1.267 | 0.159 | 0.142 | 40 | 8 | o |
| | | | | | 2-Methyl-1,3-butadiene | | | | | |
| 32-bri | 273.15 | 273.15 | 49.0 | 1176.8 | 0.568 | 0.064 | 0.041 | 14 | 2 | o |
| | | | | | 1-Pentene | | | | | |
| 51-day/fel | 353.15 | 448.15 | 0.6 | 31.6 | 0.453 | 0.090 | −0.056 | 50 | −20 | op |
| | | | | | 2-Methyl-2-butene | | | | | |
| 49-bri | 298.15 | 298.15 | 49.0 | 490.3 | 0.205 | 0.027 | 0.014 | 10 | −4 | o |
| | | | | | (*E*)-1,4-Hexadiene | | | | | |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.002 | 0.000 | 0.000 | 10 | 2 | o |
| | | | | | (2*Z*,4*E*)-2,4-Hexadiene | | | | | |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.002 | 0.000 | 0.000 | 10 | 2 | o |
| | | | | | 1,5-Hexadiene | | | | | |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.001 | 0.000 | 0.000 | 10 | −2 | o |
| | | | | | 1-Hexene | | | | | |
| 70-aba/ker | | | | | 1.279 | 0.199 | −0.492 | 160 | −62 | op |
| 72-ker/apa | 283.15 | 473.15 | 0.8 | 68.7 | 1.060 | 0.167 | −0.262 | 366 | −102 | op |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.024 | 0.004 | 0.015 | 10 | 4 | o |
| 82-gus/gal | 146.00 | 274.00 | 5.0 | 50.0 | 0.672 | 0.088 | −0.168 | 42 | −8 | o |
| | | | | | 1-Heptene | | | | | |
| 81-gus/naz | 293.15 | 353.15 | 5.0 | 50.0 | 1.162 | 0.169 | −0.165 | 23 | −7 | o |
| | | | | | 1-Octene | | | | | |
| 49-bri | | | | | 3.440 | 0.430 | −3.389 | 6 | −6 | o |
| 72-ker/apa | | | | | 3.186 | 0.486 | 0.709 | 361 | 78 | ope |
| 88-dym/mal | 298.15 | 373.15 | 10.6 | 312.7 | 0.616 | 0.082 | −0.076 | 33 | −1 | o |
| 92-naz/gas | 290.15 | 538.95 | 5.0 | 58.9 | 1.576 | 0.244 | 0.516 | 67 | 15 | op |
| | | | | | 1-Nonene | | | | | |
| 84-gus/gal | 198.00 | 398.00 | 10.0 | 50.0 | 0.694 | 0.092 | −0.018 | 44 | 0 | o |
| | | | | | 2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene | | | | | |
| 70-kus/tas | 298.15 | 353.15 | 39.2 | 196.1 | 0.098 | 0.011 | 0.002 | 20 | 4 | o |
| | | | | | Cyclopentane | | | | | |
| 69-bra/fre | | | | | 3.698 | 0.452 | 3.402 | 3 | 3 | o |
| 70-kus/tas | 313.15 | 353.15 | 39.2 | 196.1 | 1.503 | 0.185 | 0.682 | 14 | 6 | op |
| 92-bao/cac | 192.79 | 298.15 | 0.1 | 104.3 | 0.081 | 0.010 | 0.005 | 186 | 16 | o |
| | | | | | Methylcyclopentane | | | | | |
| 80-oza/ooy | 298.20 | 348.20 | 9.9 | 196.2 | 0.512 | 0.066 | −0.194 | 41 | −11 | op |
| 87-hol/goe | 293.15 | 293.15 | 2.0 | 10.0 | 0.010 | 0.001 | −0.002 | 5 | −1 | o |
| | | | | | Cyclohexane | | | | | |
| 34-rot/nag | | | | | 0.538 | 0.068 | 0.467 | 9 | 9 | o |
| 40-sch/hof | | | | | 1.753 | 0.241 | 0.308 | 3 | 1 | e |
| 57-rea/sag | | | | | 2.396 | 0.357 | 1.077 | 78 | 40 | o |
| 59-gol/vag | | | | | 3.959 | 0.697 | 1.793 | 64 | 16 | e |
| 59-gol/vag | | | | | 7.709 | 1.226 | −5.683 | 56 | −56 | op |
| 62-hol/wha | 298.16 | 348.15 | 1.0 | 10.0 | 0.008 | 0.001 | 0.005 | 50 | 34 | o |

**Table 4. 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] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Cyclohexane (continued) | | | | | |
| 70-kus/tas | | | | | 1.565 | 0.201 | −1.492 | 6 | −6 | o |
| 72-gol/ada | | | | | 6.137 | 0.763 | −5.887 | 24 | −24 | o |
| 72-ker/apa | | | | | 1.636 | 0.242 | −1.160 | 440 | −356 | op |
| 72-lys | | | | | 15.999 | 1.875 | −15.999 | 1 | −1 | o |
| 73-ker/apa | | | | | 1.455 | 0.215 | −1.107 | 272 | −212 | op |
| 73-rog/bur | 298.15 | 298.15 | 1.0 | 10.0 | 0.075 | 0.010 | −0.064 | 10 | −10 | o |
| 74-apa/ker | | | | | 2.707 | 0.426 | −1.572 | 90 | −56 | op |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.029 | 0.004 | −0.025 | 10 | −10 | o |
| 75-gri/mur | 498.15 | 523.15 | 2.1 | 79.1 | 1.046 | 0.185 | 0.322 | 28 | 14 | p |
| 75-ras/gri | 298.15 | 473.15 | 0.6 | 85.4 | 0.271 | 0.038 | 0.013 | 96 | −6 | op |
| 75-ras/gri | 298.15 | 473.15 | 1.6 | 71.0 | 0.121 | 0.017 | −0.001 | 35 | 1 | op |
| 78-gou | 314.15 | 393.15 | 5.1 | 40.1 | 0.428 | 0.057 | 0.164 | 75 | 37 | p |
| 79-dic | | | | | | | | 0 | 0 | e |
| 79-isd/dym | 298.15 | 348.15 | 10.0 | 20.0 | 0.272 | 0.035 | −0.245 | 4 | −4 | o |
| 79-isd/dym | 348.15 | 348.15 | 50.0 | 100.0 | 0.869 | 0.110 | −0.868 | 2 | −2 | o |
| 79-kas/fuk | 298.15 | 348.15 | 6.9 | 105.3 | 0.313 | 0.040 | −0.192 | 32 | −18 | o |
| 80-jon/has | 313.00 | 383.00 | 5.0 | 214.0 | 0.947 | 0.122 | −0.659 | 38 | −26 | ope |
| 82-wis/wue | 286.80 | 337.90 | 10.0 | 110.0 | 0.496 | 0.063 | −0.219 | 24 | −6 | o |
| 84-mat/van | 288.15 | 313.15 | 2.5 | 35.0 | 0.120 | 0.015 | 0.094 | 34 | 34 | o |
| 87-sun/kor | 288.15 | 323.06 | 5.0 | 85.0 | 0.260 | 0.033 | −0.233 | 80 | −80 | o |
| 88-mor/aon | 298.15 | 313.15 | 2.4 | 46.1 | 0.216 | 0.028 | −0.098 | 27 | −9 | o |
| 89-vos/slo | | | | | 3.755 | 0.563 | 3.299 | 24 | 24 | e |
| 90-pol/wei | 293.20 | 368.10 | 5.0 | 180.0 | 0.793 | 0.097 | 0.538 | 35 | 21 | o |
| 90-tos/fig | | | | | 1.787 | 0.227 | −1.483 | 48 | −40 | o |
| 90-tos/fig | | | | | 1.680 | 0.211 | −1.579 | 6 | −6 | o |
| 91-mel/mel | 293.15 | 413.15 | 10.0 | 250.0 | 1.855 | 0.234 | 0.850 | 49 | 13 | pe |
| 91-tan/hos | 298.15 | 348.15 | 6.2 | 100.0 | 0.264 | 0.034 | −0.202 | 23 | −21 | o |
| 92-lag/bon | 288.15 | 323.15 | 5.0 | 15.0 | 0.334 | 0.043 | −0.249 | 18 | −14 | o |
| 92-lag/bon | 288.15 | 323.15 | 5.0 | 15.0 | 0.331 | 0.042 | 0.229 | 18 | 14 | o |
| 96-pad/far | 298.15 | 348.14 | 5.1 | 38.0 | 0.359 | 0.047 | −0.140 | 20 | −8 | o |
| | | | | | Cyclohexane-$d_{12}$ | | | | | |
| 84-mat/van | 288.15 | 313.15 | 2.5 | 35.0 | 0.022 | 0.002 | −0.001 | 35 | −3 | o |
| | | | | | Methylcyclohexane | | | | | |
| 49-bri | | | | | 4.330 | 0.519 | −3.459 | 10 | −8 | o |
| 69-bra/fre | | | | | 1.899 | 0.216 | 0.287 | 9 | −1 | o |
| 70-aba/ker | | | | | 3.347 | 0.490 | −2.415 | 195 | −185 | op |
| 72-ker/apa | | | | | 4.305 | 0.628 | −2.446 | 351 | −331 | op |
| 72-ker/apa | 283.15 | 523.15 | 0.3 | 4.0 | 0.433 | 0.068 | −0.024 | 20 | −4 | op |
| 78-gou | 293.15 | 392.55 | 5.1 | 40.1 | 0.191 | 0.025 | 0.075 | 75 | 25 | p |
| 79-jon/has | 203.00 | 298.00 | 50.0 | 500.0 | 0.819 | 0.094 | −0.083 | 21 | −3 | o |
| 97-bay/bon | 303.15 | 343.15 | 20.0 | 40.0 | 0.351 | 0.046 | −0.157 | 6 | −2 | o |
| | | | | | Cycloheptane | | | | | |
| 70-kus/tas | 298.15 | 353.15 | 39.2 | 196.1 | 0.211 | 0.026 | −0.100 | 12 | −4 | o |
| 78-gou | 293.65 | 393.15 | 5.1 | 40.1 | 0.343 | 0.043 | 0.166 | 90 | 44 | p |
| | | | | | Ethylcyclohexane | | | | | |
| 83-gus/sha | 293.15 | 523.15 | 5.0 | 50.0 | 0.781 | 0.111 | −0.054 | 72 | −4 | op |
| 89-vos/slo | 327.10 | 440.90 | 0.4 | 9.7 | 1.022 | 0.136 | 0.502 | 21 | 13 | p |
| | | | | | 1-*cis*-2-Dimethylcyclohexane | | | | | |
| 89-vos/slo | 325.20 | 461.20 | 0.4 | 9.7 | 0.625 | 0.082 | −0.043 | 21 | −2 | p |
| | | | | | Cyclooctane | | | | | |
| 78-gou | 313.65 | 393.85 | 5.1 | 40.1 | 0.211 | 0.026 | −0.003 | 75 | −3 | p |
| | | | | | *trans*-Bicyclo[4.4.0]decane (*trans*-decalin) | | | | | |
| 70-kus/tas | 298.15 | 353.15 | 39.2 | 196.1 | 0.019 | 0.002 | 0.000 | 20 | 2 | o |
| | | | | | Butylcyclohexane | | | | | |
| 87-hol/goe | 293.15 | 293.15 | 2.0 | 10.0 | 0.003 | 0.000 | 0.000 | 5 | 1 | o |
| | | | | | Bicyclohexyl | | | | | |
| 88-sid/tej | 298.20 | 338.20 | 0.7 | 34.5 | 0.199 | 0.023 | −0.039 | 21 | −3 | o |
| | | | | | Octadecahydrochrysene | | | | | |
| 59-low/spe | 310.93 | 408.15 | 20.0 | 340.0 | 0.359 | 0.036 | −0.025 | 48 | −6 | o |
| | | | | | 1,7-Dicyclopentyl-4-(3-cyclopentylpropyl)heptane | | | | | |
| 58-cut/mcm | 310.95 | 408.15 | 34.5 | 1033.7 | 0.741 | 0.077 | 0.052 | 113 | −11 | o |
| | | | | | 1-(1-Decahydronaphthyl)pentadecane | | | | | |
| 58-cut/mcm | 333.15 | 408.15 | 34.5 | 585.7 | 0.445 | 0.049 | 0.025 | 49 | 11 | o |
| | | | | | 1-Cyclopentyl-4-(3-cyclopentylpropyl)dodecane | | | | | |
| 58-cut/mcm | 310.95 | 408.15 | 34.5 | 1033.7 | 1.209 | 0.128 | 0.070 | 149 | 3 | o |
| | | | | | 1-Cyclohexyl-3-(2-cyclohexylethyl)undecane | | | | | |
| 58-cut/mcm | 310.95 | 408.15 | 34.5 | 895.8 | 0.869 | 0.093 | 0.067 | 103 | 11 | o |

**Table 4. 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] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | 9-(2-Cyclohexylethyl)heptadecane | | | | | | |
| 58-cut/mcm | 310.95 | 408.15 | 34.5 | 1033.7 | 0.501 | 0.054 | 0.028 | 126 | 0 | o |
| | | | | 9-(3-Cyclopentylpropyl)heptadecane | | | | | | |
| 58-cut/mcm | 310.95 | 408.15 | 34.5 | 1033.7 | 0.563 | 0.062 | 0.048 | 139 | −17 | o |
| | | | | 1,1-Bis(decahydro-1-naphthyl)undecane | | | | | | |
| 59-low/spe | 310.93 | 408.15 | 20.0 | 300.0 | 0.589 | 0.062 | 0.094 | 35 | 7 | o |
| | | | | 1,3-Cyclohexadiene | | | | | | |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.002 | 0.000 | 0.000 | 10 | 0 | o |
| 79-dic | | | | | | | | 0 | 0 | |
| | | | | 1,4-Cyclohexadiene | | | | | | |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.002 | 0.000 | 0.000 | 10 | 0 | o |
| 79-dic | | | | | | | | 0 | 0 | |
| | | | | Cyclohexene | | | | | | |
| 72-ker/apa | | | | | 3.103 | 0.382 | −2.881 | 140 | −138 | o |
| 75-bur/ric | 293.15 | 298.15 | 1.0 | 5.0 | 0.012 | 0.001 | 0.001 | 10 | −2 | o |
| 79-dic | | | | | | | | 0 | 0 | |
| 91-mel/mel | 293.15 | 353.15 | 10.0 | 250.0 | 2.773 | 0.333 | −1.396 | 40 | −28 | p |

[a] o, from the same source as the compressed liquid density data; e, from the smoothing equation (see Appendix); p, extrapolated to $P_{ref}$ along isotherms using the Tait equation.

The temperature and pressure ranges of the validity of the fits given in the table allow one to avoid extrapolation using eq 1 with the parameters from Table 3 beyond the $P-T$ areas of the retained data. The $P-T$ areas that are not rectangular are shown in the figures (Figure 1), which provide crude information on the distribution of the retained data points. Nonrectangular $P-T$ areas appeared mostly for measurements where the $P-T$ range approached the vicinity of a solid−liquid equilibrium line.

Table 4 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 subsets, that is, those for which no $T$ and $P$ ranges are given in the table, illustrate the deviations of the rejected points from eq 1, but only for those values within the $P-T$ areas of the retained data (see Table 3 and Figure 1). If only one set of smoothed $P-\rho-T$ values available in original sources (S-type data) or one set of values generated from published equations (F-type data) for a particular substance was fitted by eq 1, then the average deviations of the fit (RMSD, RMSD$_r$) do not reflect the real accuracy of the experiment and consequently the weighted standard deviation $s_w$ may be lower than unity (the deviations of both the smoothed input data and the F-type data from eq 1 are lower than the experimental uncertainty declared by the authors).

Values at high temperatures of some retained data sets were rejected in those cases where large deviations from the Tait equation were observed and it was not possible to improve the fit by the additional parameters $b_i$ and $c_i$. Thus, the $P-T$ ranges of some fits do not cover the entire original range of retained data sets. The temperature and/or pressure ranges were sometimes enlarged by retaining less accurate and less reliable values in the ranges beyond those of more accurate data sets but only in those cases where the representation of accurate data was not affected by the enlargement and the enlargement did not result in a distortion of the $B(T)$ function. The absence of extremes and inflection points on the function $B(T)$ (eq 3) of all final fits was checked.

A comparison of isothermal compressibilities, $\beta_T = -(1/V)(\partial V/\partial P)_T = (1/\rho)(\partial\rho/\partial P)_T$, calculated from the fits for $P =$ 0.1 MPa with available values published in the literature is presented in Table 5, which provides a rough check of the consistency of the fits with independent data. The literature values of isothermal compressibility used for the comparison in Table 5 are the values obtained mostly from speed-of-sound measurements and were either taken directly from the papers or calculated from the equation

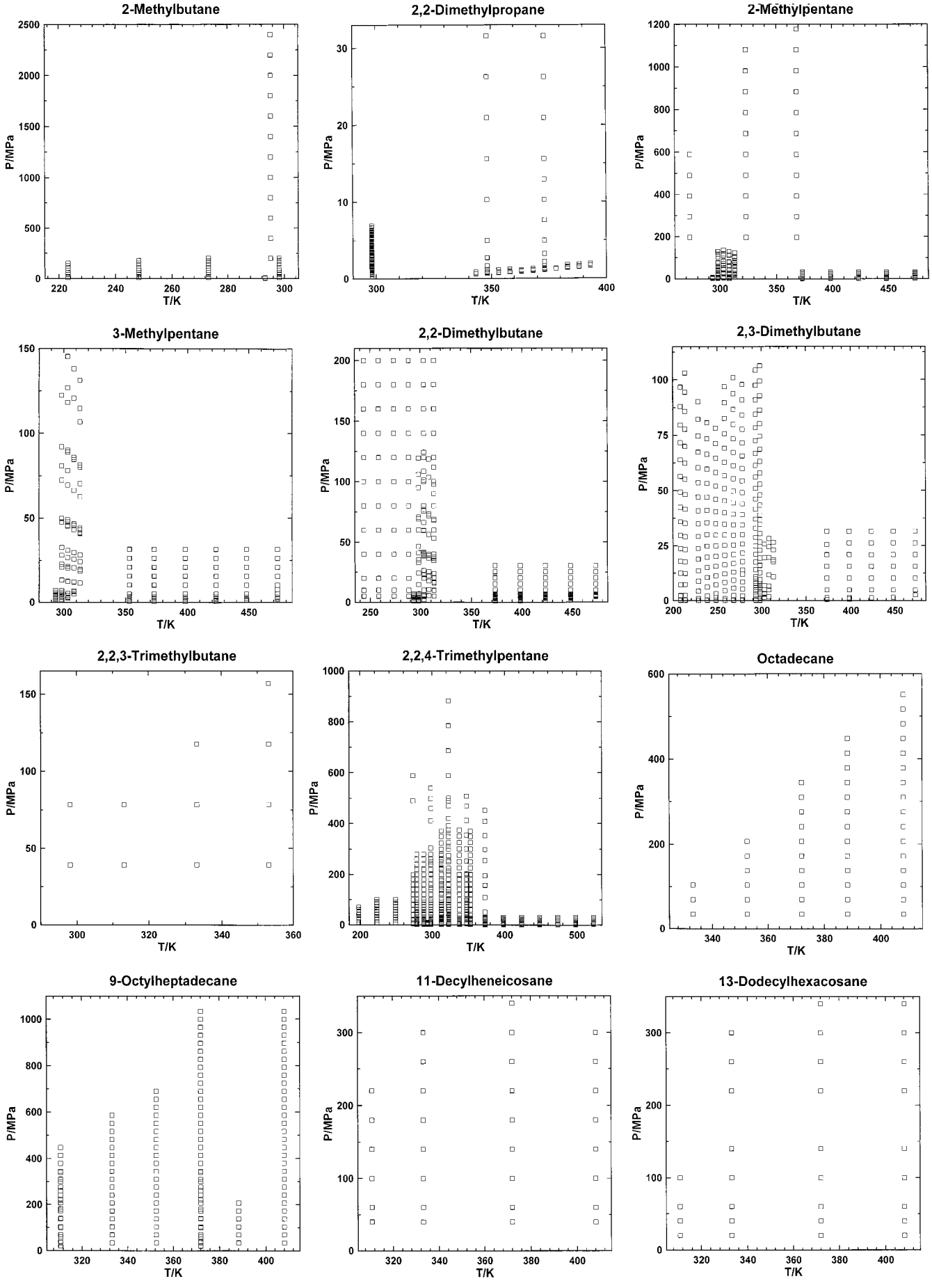
$$\beta_T = \frac{1}{\rho}\left[\frac{1}{u^2} + \frac{TM\alpha_p^2}{c_p}\right] \tag{11}$$

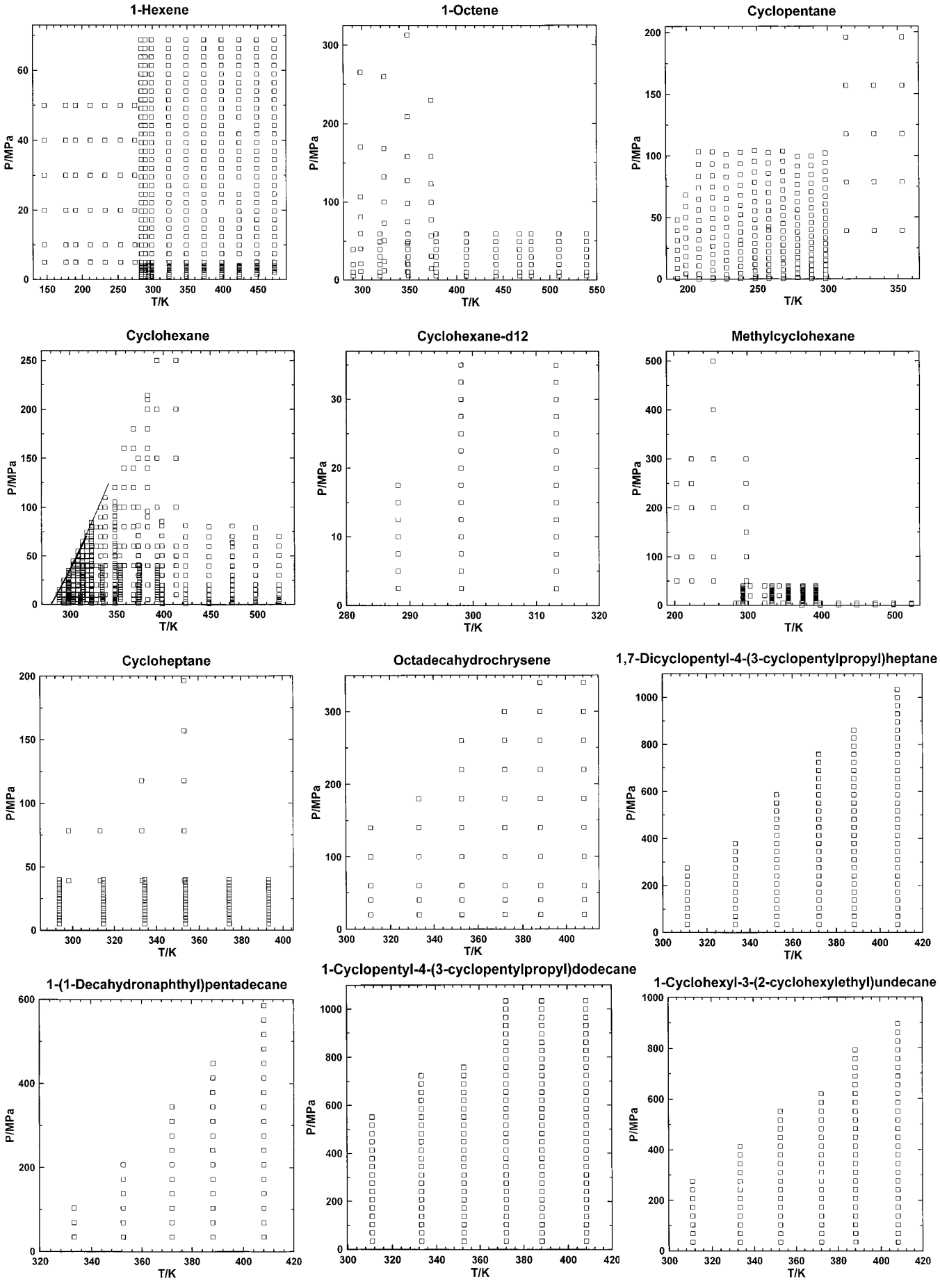
where $M$, $u$, $\alpha_P$, and $c_P$ are the molar mass, speed of sound, isobaric thermal expansivity ($\alpha_P = (1/V)(\partial V/\partial T)_P = -(1/\rho)(\partial\rho/\partial T)_P$), and molar isobaric heat capacity, respectively. The values of the input quantities in eq 11 were taken from the different sources cited in Table 5.

***Alkanes.*** Data [92-wal/bar] for 2-methylbutane in the low-temperature range differ from those by Mopsik [69-mop]. Tentative fits of each of those data sets revealed that the data of Mopsik [69-mop] gave much better agreement (positive deviations about 1% on average) with isothermal compressibilities evaluated from speed of sound [92-wal/bar] than with $P-\rho-T$ data [92-wal/bar] (negative deviations in the range from −1.6% at 203 K to −12.2% at 243 K). The final fit yields the average deviation in the isothermal compressibility 2% (positive, see Table 5), even when the values extrapolated beyond the temperature range of the fit are included.

The agreement between the calculated and experimental isothermal compressibilities of 2-methylpentane is satisfactory (deviation 1.8% on average) at temperatures where the fit represents the data of Sahli et al. and Moriyoshi and Aono [76-sah/gag, 88-mor/aon] while a larger deviation (−4.3%) is observed at 273.15 K where the fit is based on less accurate data by Bridgman [31-bri]. Bridgman's data were, however, rejected for $P < 196$ MPa.

The average deviations of the data retained for 3-methylpentane and 2,2-dimethylbutane from the final fits (Table 3) are within 0.1%, and the average deviations of the isothermal compressibilities (Table 5) are 0.5 and 1.9%, respectively. The deviation of the isothermal compressibility extrapolated from the fit for 3-methylpentane is 5.1% at 273.15 K (20 K below $T_{min}$ of the fit); much better agreement (1.4%) is observed for $T = 283.15$ K.


2-Methylbutane
2,2-Dimethylpropane
2-Methylpentane
3-Methylpentane
2,2-Dimethylbutane
2,3-Dimethylbutane
2,2,3-Trimethylbutane
2,2,4-Trimethylpentane
Octadecane
9-Octylheptadecane
11-Decylheneicosane
13-Dodecylhexacosane
P/MPa
T/K


1-Hexene
P/MPa
T/K
1-Octene
P/MPa
T/K
Cyclopentane
P/MPa
T/K
Cyclohexane
P/MPa
T/K
Cyclohexane-d12
P/MPa
T/K
Methylcyclohexane
P/MPa
T/K
Cycloheptane
P/MPa
T/K
Octadecahydrochrysene
P/MPa
T/K
1,7-Dicyclopentyl-4-(3-cyclopentylpropyl)heptane
P/MPa
T/K
1-(1-Decahydronaphthyl)pentadecane
P/MPa
T/K
1-Cyclopentyl-4-(3-cyclopentylpropyl)dodecane
P/MPa
T/K
1-Cyclohexyl-3-(2-cyclohexylethyl)undecane
P/MPa
T/K

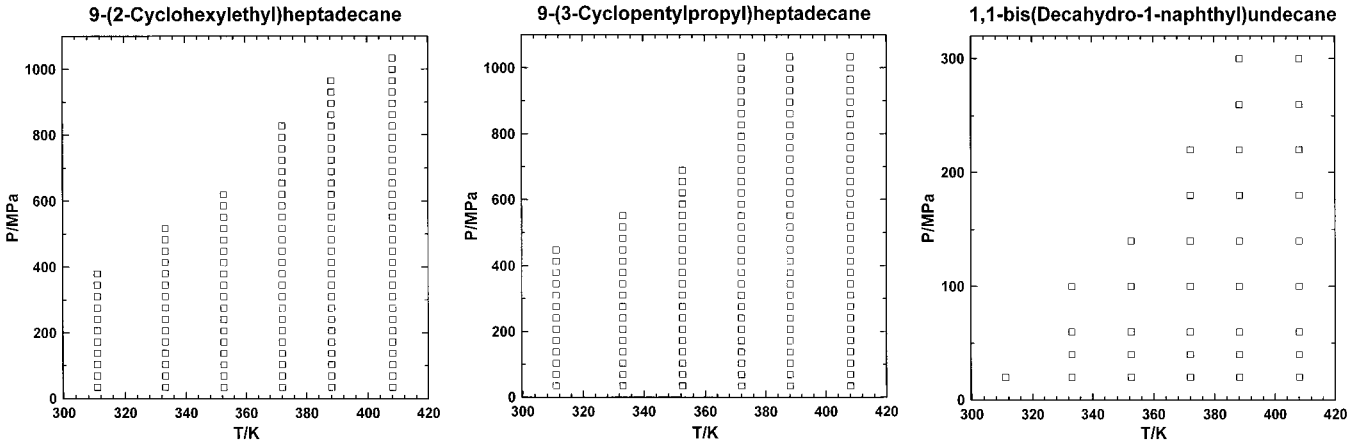



**Figure 1.** Temperature and pressure coordinates of data points retained in the correlations for the fits in Table 3 where $P-T$ areas of retained data points are not rectangular. The lines represent solid−liquid equilibrium curves; cyclohexane (normal melting temperature 279.6 K): [75-ras/gri] {up to 318 K (70 MPa)}, [82-wis/wue] {up to 338 K (117 MPa)}, [93-yok/ebi] {up to 341 K (122 MPa)}.

Two fits are presented for 2,3-dimethylbutane. The first one, performed in as wide a temperature range as possible, yielded isothermal compressibilities 2.4% higher than the available literature values (Table 5); the second fit, representing data [76-sah/gag, 87-hol/goe, 88-mor/aon] in the range 293.15−313.15 K, is in perfect agreement with experimental data on isothermal compressibilities. Data [90-rie/sch] exhibit large deviations and were rejected in both cases. From the comparison of both fits (Table 4), it, however, follows that the values of Baonza et al. [93-bao/cac] are in the range 293.15−298.15 K, lower than other data retained for the narrow-temperature-range fit.

Fits of the data of Kuss and Taslimi [70-kus] for 3-ethylpentane and 2,2,3-trimethylbutane yielded similar deviation from available isothermal compressibilities (within 6%). The fit for 2,2-dimethylpentane is the fit of the F-type data of Sahli et al. [76-sah/gag]; the agreement for the isothermal compressibility is very good.

The fit for 2,2,4-trimethylpentane covers a temperature range more than 300 K wide. The experimental data are in good agreement, and few data sets were rejected (Table 4). The average deviation of the isothermal compressibility in the range 233.15−318.15 K is excellent, being 1.2%. Values reported in [96-pad/far-1] for the temperature range 298−348 K represent the same "raw" data as those from [94-pad/far], but they were analyzed by Padua and coworkers using a theoretically improved model of the vibrating-wire densimeter. It was, however, found that the fit of the values of [94-pad/far] gives much better agreement with available isothermal compressibilities at 0.1 MPa than that of the values of [96-pad/far-1] (average deviation −2.5% in the range 233−318 K). Therefore, both sets of density values were retained in the correlations, each with its declared uncertainty (0.1% for [94-pad/far], 0.05% for [96-pad/far-1]).

Fits for other alkanes are mostly fits of a set of data from one source. Except for dodecane, where large deviations from literature values are observed, the data to obtain independent isothermal compressibilities for comparison were not available. The data along the the isotherm 388.15 K for 9-octylheptadecane [58-cut/mcm] were rejected to obtain satisfactory consistency with the data from the same laboratory [59-low/spe]. The data along the isobars 20 MPa of 11-decylheneicosane (negative deviations 3−5 kg·m$^{-3}$) and 180 MPa of 13-dodecylhexacosane (positive deviations 1.8−2.4 kg·m$^{-3}$) were rejected.

***Alkenes.*** The upper temperature limit of the data for 1-pentene is 448.15 K; the authors [51-day/fel] declared that observable polymerization of the substance occurred at temperatures higher than 473 K. The data for 1-hexene cover the temperature range up to 503 K. No polymerization was mentioned by the authors, but the fit was limited up to 473.15 K, since large deviations were observed for higher temperatures. Agreement of the isothermal compressibilities calculated from the fit for 293.15 and 298.15 K is very good (Table 5).

Similarly the upper temperature limit of the fit for 1-heptene is 353 K while the data covers temperatures up to 523 K. When the temperature range of the correlation was increased, points of inflection and even local extremes appeared on the function $B(T)$. The isothermal compressibilities calculated from the final fit are 19% lower than experimental values. Similar results were reached in the case of the data for 1-nonene from the same laboratory [84-gus/gal]; the temperature range of the final fit was limited up to 398 K; the deviations in isothermal compressibilities are −26%. It is worth mentioning that the values of the Tait parameters $c_i$, and $b_i$ for these two alkenes (Table 3) seem to be rather unusual.

The fit for 1-octene represents the data of Dymond et al. [88-dym/mal] and Naziev et al. [92 naz/gas]. Rather large deviations were observed for the data of Naziev et al. [92-naz/gas]., but the increase of the number of adjustable parameters led to distortion of the $B(T)$ function. The agreement of the isothermal compressibilities calculated from the final fit with literature values is satisfactory.

***Cycloalkanes.*** The fit for cyclopentane represents predominantly of data of Baonza et al. [92-bao/cac]; the temperature range of the fit was extended by retaining the data of Kuss and Taslimi [70-kus/tas] The calculated isothermal compressibilities agree with the literature values within 2% (neglecting the less accurate value of Shinoda and Hildebrand [61-shi/hil]).

The fit for cyclohexane covers the temperature range from a few Kelvins above the normal melting point (279.6 K) up to 30 K below the critical temperature. The deviations of the calculated isothermal compressibility from literature data are very satisfactory, being about 1.5% in the temperature interval 293 to 352 K (see Table 5). Several data sets for cyclohexane present values at higher temperatures. Among them, the data of Grigoriev et al. [75-gri/mur, 75-ras/gri] were retained, since much better agreement with other retained data was observed at lower temperatures for these data than for the values of Kerimov et al. [72-ker/apa, 73-ker/apa, 74-apa/ker]. This is in accordance with the results of Penoncello et al. [95-pen/

**Table 5. Comparison of Values of Isothermal Compressibility, $\beta_T = (1/\rho)(\partial\rho/\partial P)_T$, at $P = 0.1$ MPa Calculated from the Fits in Table 3 (Eq 1) with Literature Data**

| $T$/K | $\beta_T$/GPa$^{-1}$ eq 1[a] | $\beta_T$/GPa$^{-1}$ lit. | $\delta\beta_T$/% [b] | ref(s) | $T$/K | $\beta_T$/GPa$^{-1}$ eq 1[a] | $\beta_T$/GPa$^{-1}$ lit. | $\delta\beta_T$/% [b] | ref(s) |
|---|---|---|---|---|---|---|---|---|---|
| | | | | 2-Methylbutane | | | | | |
| 203.00 | 0.911[i] | 0.893 | 2.0 | 92-wal/bar,[d] 96-trc,[e] 96-zab/ruz[f] | 233.00 | 1.198 ± 0.006 | 1.168 | 2.6 | 92-wal/bar,[d] 96-trc,[e] 96-zab/ruz[f] |
| 213.00 | 0.996[i] | 0.977 | 1.9 | 92-wal/bar,[d] 96-trc,[e] 96-zab/ruz[f] | 243.00 | 1.320 ± 0.006 | 1.291 | 2.2 | 92-wal/bar,[d] 96-trc,[e] 96-zab/ruz[f] |
| 223.00 | 1.092 ± 0.007 | 1.073 | 1.8 | 92-wal/bar,[d] 96-trc,[e] 96-zab/ruz[f] | | | | | |
| | | | | 2-Methylpentane | | | | | |
| 273.15 | 1.415 ± 0.012 | 1.479 | −4.3 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] | 298.15 | 1.793 ± 0.007 | 1.807 | −0.8 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] |
| 283.15 | 1.551 ± 0.009 | 1.595 | −2.7 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] | | | 1.833 | −2.2 | 89-ohn/fuj[c] |
| 298.15 | 1.793 ± 0.007 | 1.839 | −2.5 | 83-aic/kum,[c] 88-tre/ben[c] | 313.15 | 2.091 ± 0.008 | 2.072 | 0.9 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] |
| | | | | 3-Methylpentane | | | | | |
| 273.15 | 1.392[i] | 1.325 | 5.1 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] | 298.15 | 1.714 ± 0.006 | 1.719 | −0.3 | 83-aic/kum,[c] 88-tre/ben[c] |
| 283.15 | 1.508[i] | 1.486 | 1.4 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] | | | 1.699 | 0.9 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] |
| 293.15 | 1.641 ± 0.007 | 1.627 | 0.9 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] | | | 1.714 | 0.0 | 89-ohn/fuj[c] |
| | | | | | 313.15 | 1.966 ± 0.007 | 1.970 | −0.2 | 83-aww/pet,[d] 92-trc,[e] 96-zab/ruz[f] |
| | | | | 2,2-Dimethylbutane | | | | | |
| 298.15 | 1.967 ± 0.008 | 2.014 | −2.3 | 82-tre/han[c] | 298.15 | 1.967 ± 0.008 | 1.997 | −1.5 | 85-cos/bha[c] |
| | | 2.010 | −2.1 | 83-aic/kum,[c] 88-tre/ben[c] | | | 2.002 | −1.7 | 89-ohn/fuj[c] |
| | | | | 2,3-Dimethylbutane | | | | | |
| 298.15 | 1.831 ± 0.006 | 1.790 | 2.3 | 83-aic/kum,[c] 88-tre/ben[c] | 298.15 | 1.831 ± 0.006 | 1.786 | 2.5 | 89-ohn/fuj[c] |
| 298.15 | 1.787 ± 0.006[g] | 1.790 | −0.2 | 83-aic/kum,[c] 88-tre/ben[c] | 298.15 | 1.787 ± 0.006[g] | 1.786 | 0.05 | 89-ohn/fuj[c] |
| | | | | 3-Ethylpentane | | | | | |
| 318.15 | 1.606 ± 0.007 | 1.701 | −5.6 | 29-fre/hub,[d] 91-trc-1,[e] 96-zab/ruz[f] | | | | | |
| | | | | 2,2-Dimethylpentane | | | | | |
| 293.15 | 1.569 ± 0.004 | 1.604 | −2.2 | 29-fre/hub,[d] 91-trc-1,[e] 96-zab/ruz[f] | 298.15 | 1.667 ± 0.004 | 1.660 | 0.4 | 84-aww/pet,[d] 91-trc-1,[e] 96-zab/ruz[f] |
| | | | | 2,2,3-Trimethylbutane | | | | | |
| 298.15 | 1.482 ± 0.006 | 1.566 | −5.4 | 88-tre/ben[c] | 318.15 | 1.781 ± 0.007 | 1.717 | 3.7 | 29-fre/hub,[d] 91-trc-1,[e] 96-zab/ruz[f] |
| | | | | 2,2,4-Trimethylpentane | | | | | |
| 233.15 | 0.942 ± 0.006 | 0.924 | 1.9 | 83-aww/pet,[d] 90-trc,[e] 96-zab/ruz[f] | 298.15 | 1.535 ± 0.002 | 1.546 | −0.7 | 91-pap/zia,[d] 90-trc,[e] 96-zab/ruz[f] |
| 253.15 | 1.089 ± 0.004 | 1.068 | 2.0 | 83-aww/pet,[d] 90-trc,[e] 96-zab/ruz[f] | | | 1.541 | −0.4 | 94-ami/ara,[d] 90-trc,[e] 96-zab/ruz[f] |
| 263.15 | 1.172 ± 0.003 | 1.157 | 1.3 | 83-aww/pet,[d] 90-trc,[e] 96-zab/ruz[f] | | | 1.563 | −1.8 | 95-mie/osw[c] |
| 273.15 | 1.264 ± 0.002 | 1.259 | 0.4 | 83-aww/pet,[d] 90-trc,[e] 96-zab/ruz[f] | | | 1.550 | −1.0 | 95-ami/gop,[d] 90-trc,[e] 96-zab/ruz[f] |
| 293.15 | 1.475 ± 0.002 | 1.471 | 0.3 | 83-aww/pet,[d] 90-trc,[e] 96-zab/ruz[f] | 308.15 | 1.664 ± 0.003 | 1.678 | −0.8 | 94-ami/ara,[d] 90-trc,[e] 96-zab/ruz[f] |
| 298.15 | 1.535 ± 0.002 | 1.56 | −1.6 | 61-shi/hil[c] | 313.15 | 1.734 ± 0.003 | 1.774 | −2.3 | 95-mie/osw[c] |
| | | 1.542 | −0.5 | 82-tre/han,[c] 88-tre/ben,[c] 85-cos/bha[c] | 318.15 | 1.808 ± 0.003 | 1.844 | −2.0 | 29-fre/hub,[d] 90-trc,[e] 96-zab/ruz[f] |
| | | 1.543 | −0.5 | 83-aww/pet,[d] 90-trc,[e] 96-zab/ruz[f] | | | 1.834 | −1.4 | 94-ami/ara,[d] 90-trc,[e] 96-zab/ruz[f] |
| | | | | Docosane | | | | | |
| 323.15 | 1.02 ± 0.07 | 0.900 | 13.3 | 82-bro/lop[h] | 353.15 | 1.36 ± 0.10 | 1.066 | 27.2 | 82-bro/lop[h] |
| 333.15 | 1.14 ± 0.07 | 0.950 | 19.7 | 82-bro/lop[h] | 363.15 | 1.45 ± 0.11 | 1.130 | 27.6 | 82-bro/lop[h] |
| 343.15 | 1.26 ± 0.08 | 1.006 | 25.2 | 82-bro/lop[h] | | | | | |
| | | | | 1-Hexene | | | | | |
| 293.15 | 1.589 ± 0.005 | 1.584 | 0.3 | 58-par/pan,[d] 95-trc,[e] 96-zab/ruz[f] | 298.15 | 1.666 ± 0.005 | 1.689 | −1.4 | 86-tar/dia[c] |
| 298.15 | 1.666 ± 0.005 | 1.614 | 3.2 | 75-bur/ric[c] | | | | | |
| | | | | 1-Heptene | | | | | |
| 283.15 | 1.06[i] | 1.289 | −17.8 | 48-lag/mcm,[d] 95-trc-1,[e] 96-zab/ruz[f] | 303.15 | 1.27 ± 0.07 | 1.577 | −19.5 | 48-lag/mcm,[d] 95-trc-1,[e] 96-zab/ruz[f] |
| 293.15 | 1.16 ± 0.06 | 1.437 | −19.3 | 48-lag/mcm,[d] 95-trc-1,[e] 96-zab/ruz[f] | | | | | |
| | | | | 1-Octene | | | | | |
| 283.15 | 1.215[i] | 1.162 | 4.6 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] | 293.15 | 1.285[i] | 1.243 | 3.4 | 58-par/pan[c] |
| 293.15 | 1.285[i] | 1.259 | 2.1 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] | 303.15 | 1.361 ± 0.010 | 1.354 | 0.5 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] |
| | | | | 1-Nonene | | | | | |
| 283.15 | 0.79 ± 0.02 | 1.067 | −26.0 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] | 298.15 | 0.88 ± 0.02 | 1.182 | −25.5 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] |
| 293.15 | 0.85 ± 0.02 | 1.145 | −25.8 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] | 303.15 | 0.91 ± 0.03 | 1.229 | −26.0 | 48-lag/mcm,[d] 86-trc,[e] 96-zab/ruz[f] |
| | | | | Cyclopentane | | | | | |
| 298.15 | 1.308 ± 0.006 | 1.35 | −3.1 | 61-shi/hil[c] | 298.15 | 1.308 ± 0.006 | 1.332 | −1.8 | 86-tar/dia[c] |
| | | 1.331 | −1.7 | 74-ewi/mar,[c] 77-ewi/mar[c] | 303.15 | 1.369 ± 0.006 | 1.379 | −0.7 | 49-wei,[d] 95-trc-3,[e] 96-zab/ruz[f] |
| | | | | Cyclohexane | | | | | |
| 292.85 | 1.086 ± 0.002 | 1.051 | 3.3 | 85-lav/jak,[d] 91-trc,[e] 96-zab/ruz[f] | 298.15 | 1.135 ± 0.002 | 1.113 | 2.0 | 95-ami/gop,[d,e] 96-zab/ruz[f] |
| 293.15 | 1.089 ± 0.002 | 1.038 | 4.9 | 52-jac[c] | 303.15 | 1.184 ± 0.002 | 1.145 | 3.4 | 85-lav/jak,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.080 | 0.8 | 71-ric/rog[c] | | | 1.174 | 0.9 | 85-tam/mur,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.096 | −0.6 | 75-bur/ric[c] | | | 1.169 | 1.3 | 90-sek/ven[c] |
| | | 1.069 | 1.9 | 85-mar/bha,[d] 91-trc,[e] 96-zab/ruz[f] | | | 1.220 | −3.0 | 95-osw/pat[c] |
| | | 1.076 | 1.2 | 85-tam/mur,[d] 91-trc,[e] 96-zab/ruz[f] | 308.15 | 1.236 ± 0.001 | 1.219 | 1.4 | 80-aic/tar,[c] 81-aic/tar,[c] 81-aic/tar-1[c] |
| 298.15 | 1.135 ± 0.002 | 1.130 | 0.4 | 61-shi/hil,[c] 72-ewi/mar,[c] 78-kiy/hal[c] | | | 1.218 | 1.5 | 83-nat/tri,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.155 | −1.7 | 74-jai/nor,[d] 91-trc,[e] 96-zab/ruz[f] | 313.15 | 1.291 ± 0.001 | 1.301 | −0.8 | 63-brz/har[c] |
| | | 1.142 | −0.6 | 75-bur/ric[c] | 318.15 | 1.348 ± 0.001 | 1.331 | 1.3 | 80-aic/tar,[c] 81-aic/tar,[c] 81-aic/tar-1[c] |
| | | 1.126 | 0.8 | 78-gro/wil[c] | 318.35 | 1.351 ± 0.001 | 1.335 | 1.2 | 85-lav/jak,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.120 | 1.3 | 80-aic/tar,[c] 81-aic/tar,[c] 81-aic/tar-1[c] | 323.15 | 1.410 ± 0.001 | 1.414 | −0.3 | 63-brz/har[c] |
| | | 1.124 | 1.0 | 83-nat/tri,[d] 85-tam/mur,[d] 95-fuj/tam,[d] 91-trc,[e] 96-zab/ruz[f] | 333.15 | 1.543 ± 0.001 | 1.540 | 0.2 | 63-brz/har[c] |
| | | | | | | | 1.520 | 1.5 | 80-aic/tar,[c] 81-aic/tar,[c] 81-aic/tar-1[c] |
| | | 1.128 | 0.6 | 85-cos/bha[c] | 337.95 | 1.613 ± 0.002 | 1.573 | 2.5 | 85-lav/jak,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.120 | 1.3 | 85-mar/bha,[d] 91-trc,[e] 96-zab/ruz[f] | 343.15 | 1.693 ± 0.002 | 1.679 | 0.8 | 63-brz/har[c] |
| | | 1.129 | 0.5 | 87-oho/tam,[c] 83-tam/oho,[c] 97-oho/tam[c] | 352.05 | 1.844 ± 0.002 | 1.885 | −2.2 | 85-lav/jak,[d] 91-trc,[e] 96-zab/ruz[f] |

**Table 5. (Continued)**

| T/K | $\beta_T$/GPa$^{-1}$ eq 1[a] | $\beta_T$/GPa$^{-1}$ lit. | $\delta\beta_T$/%[b] | ref(s) | T/K | $\beta_T$/GPa$^{-1}$ eq 1[a] | $\beta_T$/GPa$^{-1}$ lit. | $\delta\beta_T$/%[b] | ref(s) |
|---|---|---|---|---|---|---|---|---|---|
| | | | | Methylcyclohexane | | | | | |
| 293.15 | 1.082 ± 0.005 | 1.108 | −2.3 | 85-tam/mur,[d] 91-trc,[e] 96-zab/ruz[f] | 298.15 | 1.126 ± 0.005 | 1.181 | −4.6 | 97-oho/tam[c] |
| 298.15 | 1.126 ± 0.005 | 1.16 | −2.9 | 61-shi/hil[c] | 303.15 | 1.172 ± 0.005 | 1.198 | −2.2 | 74-rao/nai,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.152 | −2.3 | 85-tam/mur,[d] 91-trc,[e] 96-zab/ruz[f] | | | 1.197 | −2.1 | 85-tam/mur,[d] 91-trc,[e] 96-zab/ruz[f] |
| | | 1.175 | −4.2 | 87-oho/tam[c] | | | | | |
| | | | | Cyclooctane | | | | | |
| 298.15 | 0.798[i] | 0.803 | −0.6 | 74-ewi/mar,[c] 77-ewi/mar[c] | 303.00 | 0.822[i] | 0.829 | −0.8 | 74-jai/nor,[d]70-ewi/lev,[e] 74-ewi/mar,[e] 96-zab/ruz[f] |
| | | | | *trans*-Bicyclo[4.4.0]decane | | | | | |
| 298.15 | 0.735 ± 0.001 | 0.724 | 1.5 | 85-let/bax[c] | 298.15 | 0.735 ± 0.001 | 0.764 | −3.8 | 89-ohn/fuj[c] |
| | | | | Bicyclohexyl | | | | | |
| 298.15 | 0.65 ± 0.02 | 0.674 | −3.6 | 86-tar/dia[c] | | | | | |
| | | | | 1,3-Cyclohexadiene | | | | | |
| 293.15 | 0.962 ± 0.002 | 0.968 | −0.6 | 75-bur/ric[c] | 298.15 | 1.007 ± 0.002 | 0.962 | 4.6 | 86-tar/dia[c] |
| 298.15 | 1.007 ± 0.002 | 1.012 | −0.5 | 75-bur/ric[c] | | | | | |
| | | | | 1,4-Cyclohexadiene | | | | | |
| 293.15 | 0.853 ± 0.002 | 0.862 | −1.0 | 75-bur/ric[c] | 298.15 | 0.908 ± 0.002 | 0.944 | −3.8 | 86-tar/dia[c] |
| 298.15 | 0.908 ± 0.002 | 0.917 | −1.0 | 75-bur/ric[c] | | | | | |
| | | | | Cyclohexene | | | | | |
| 293.15 | 0.993 ± 0.016 | 1.010 | −1.7 | 44-sch,[d] 72-ker/apa,[e] 96-zab/ruz[f] | 298.15 | 1.043 ± 0.016 | 1.036 | −0.7 | 86-tar/dia[c] |
| | | 0.983 | −1.0 | 75-bur/ric[c] | 303.15 | 1.096 ± 0.018 | 1.096 | −0.0 | 49-wei,[d] 72-ker/apa,[e] 96-zab/ruz[f] |
| 298.15 | 1.043 ± 0.016 | 1.041 | −0.2 | 75-bur/ric[c] | | | 1.077 | −1.8 | 90-sek/ven[d,e] 96-zab/ruz[f] |

[a] Uncertainty is estimated as ±2*s*, where *s* is a standard deviation derived from a covariance matrix of each fit. [b] $[\beta_T(\text{eq 1}) - \beta_T(\text{lit})]\cdot 100/\beta_T(\text{lit})$. [c] Isothermal compressibility, $\beta_T = -(1/V)(\partial V/\partial P)_T$. [d] Sound speed. [e] Density and thermal expansivity, $\alpha_P = (1/V)(\partial V/\partial T)_P$. [f] Isobaric heat capacity. [g] Narrow temperature range fit (see Table 4). [h] Literature values calculated from smoothing equation representing data [67-orw/flo]. [i] Extrapolated beyond the temperature range of the fit (Table 3).

jac], who selected the $P-\rho-T$ data measured by Grigoriev's group [75-gri/mur, 75-ras/gri] in deriving the fundamental equation (Helmholz energy) for cyclohexane based on various experimental property data.

The data available for methylcyclohexane are not in good mutual agreement. The selection of the data sets retained for the final fit and setting statistical weights was influenced by comparisons of isothermal compressibilities calculated from repeated fits with literature data. The final fit gives compressibilities on average 2.9% lower than available values in the range 293−303 K.

One or two data sets were available for other cycloalkanes. For some of them isothermal compressibility data were available for comparison (cyclooctane, *trans*-bicyclo-[4.4.0]decane, bicyclohexyl) and deviations below 4% were observed (Table 5). It should be mentioned that the accuracy of the density data presented by Voss and Sloan [89-vos/slo] (cyclohexane, ethylcyclohexane, *cis*-1,2-dimethylcyclohexane) is declared by the authors to be unusually low, being 2%.

***Cycloalkenes.*** The fits for 1,3-cyclohexadiene and 1,4-cyclohexadiene are recorrelations of F-type data calculated from equations presented by Burkat and Richard [75-bur/ric]. Naturally, the agreement of calculated isothermal compressibilities with values from the same source is within 1%. Larger deviations are observed for the literature values of Tardajos et al. [86-tar/dia].

The data of Melikhov et al. [91-mel/mel] for cyclohexene agree with those of Burkat and Richard [75-bur/ric] slightly better than the rejected data of Kerimov and Apaev [72-ker/apa] (see also cyclohexane); however, the average deviation of the data of Melikhov et al. [91-mel/mel] from the fit is over 0.3% (Table 4). The average deviation in the isothermal compressibility in the range 293−303 K is 0.9%.

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## Appendix: Representation of Reference Density Data $\rho[T,P_{ref}(T)] = \rho(T)$

The functions of temperature selected to represent reference density data $\rho[T, P_{ref} = 0.101325\ \text{MPa}$ or $P_{ref} = P_{sat}(T)] = \rho(T)$ are as follows

$$\rho(T/\text{K})/(\text{kg}\cdot\text{m}^{-3}) = \rho_c\{1 + \sum_{i=0}^{5} a_i(1 - T_r)^{(i+1)/3}\}, \quad T_r = T/T_c \quad \text{(A1)}$$

$$\rho(T/\text{K})/(\text{kg}\cdot\text{m}^{-3}) = \sum_{i=0}^{2} a_i(T/100)^i \quad \text{(A2)}$$

The values of the adjustable parameters $a_i$ obtained by fitting to selected data using a weighted least-squares method are recorded in Table 6 along with some characteristics of the fits. The results in Table 6 are mostly the fits of recommended values available in *Thermodynamics Research Center Thermodynamic Tables—Hydrocarbons* (TRC Tables) combined in several cases with data either presented by authors of density data at elevated pressures or obtained by extrapolation to the reference pressure. The statistical weights of density values taken from TRC Tables were related to the number of significant digits presented in the TRC Tables; in other cases the weights were estimated from information in original papers or related to the average deviations of the extrapolations. The absence of extremes and inflection points on the function $\rho(T)$ was checked for all fits. Equation A1 was preferably used in those cases where respective critical parameters ($\rho_c$, $T_c$) were available and the data covered a wide temperature range to enlarge the use of the fits beyond the temperature range of the data, particularly in the region between $T_{max}$ and $T_c$. Therefore, the fits by eq A1 with $a_0 > 0$ were

**Table 6. Parameters $a_i$ of Smoothing Functions A1 or A2 Fitted to Selected Density Values, $\rho[T,P=0.1\ \text{MPa}\ \text{or}\ P_{sat}(T)]$, Critical Densities[a] ($\rho_c$), Critical Temperatures[a] ($T_c$), Temperature Ranges of Density Data ($T_{min}$ and $T_{max}$), and RMSD of the Fits**

| eq | $a_0$ | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ | $\rho_c$/ kg·m$^{-3}$ | $T_c$/K | $T_{min}$/K | $T_{max}$/K | RMSD/ kg·m$^{-3}$ | ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | 2-Methylbutane | | | | | | | |
| A1 | 2.019558 | −1.592068 | 6.829264 | −8.866790 | 4.405885 | | 235.785 | 460.43 | 113.26 | 443.15 | 0.322 | 96-trc |
| | | | | | 2,2-Dimethylpropane | | | | | | | |
| A1 | 1.146314 | 3.273773 | −4.781257 | 3.136329 | | | 238.120 | 433.78 | 256.58 | 413.15 | 0.123 | 96-trc |
| | | | | | 2-Methylpentane | | | | | | | |
| A1 | 5.722272 | −28.29310 | 78.058688 | −90.89560 | 39.000958 | | 234.815 | 497.50 | 273.15 | 473.15 | 0.425 | 92-trc |
| | | | | | 3-Methylpentane | | | | | | | |
| A1 | 4.031489 | −11.82482 | 24.255863 | −18.32954 | 4.334045 | | 234.815 | 504.50 | 293.15 | 473.15 | 0.703 | 92-trc |
| | | | | | 2,2-Dimethylbutane | | | | | | | |
| A1 | 1.514059 | 2.294405 | −3.185144 | 2.087656 | | | 240.048 | 488.78 | 263.15 | 473.15 | 0.655 | 92-trc |
| | | | | | 2,3-Dimethylbutane[b] | | | | | | | |
| A1 | 1.515081 | 2.028384 | −2.293512 | 1.430761 | | | 240.718 | 499.98 | 207.93 | 463.15 | 0.273 | 93-bao/cac, 92-trc |
| | | | | | 3-Ethylpentane | | | | | | | |
| A1 | 34.474530 | −176.7741 | 359.19912 | −321.2713 | 107.54832 | | 240.875 | 540.64 | 273.15 | 413.15 | 0.168 | 91-trc-1 |
| | | | | | 2,2-Dimethylpentane | | | | | | | |
| A1 | 2.111867 | 1.260332 | −3.513467 | 3.029976 | | | 240.875 | 520.50 | 273.15 | 353.15 | 0.011 | 91-trc-1 |
| | | | | | 2,2,3-Trimethylbutane | | | | | | | |
| A1 | 5.668622 | −9.498036 | 6.609025 | | | | 251.769 | 531.17 | 298.15 | 353.15 | 0.686 | 91-trc-1 |
| | | | | | 2,2,4-Trimethylpentane | | | | | | | |
| A1 | 1.983676 | −1.937998 | 10.308726 | −17.09974 | 12.135390 | −2.5519 | 244.083 | 543.96 | 173.15 | 541.15 | 0.254 | 90-trc |
| | | | | | Heptadecane | | | | | | | |
| A1 | 0.973342 | 3.647183 | −4.409424 | 2.744414 | | | 246.134 | 735.00 | 293.15 | 613.15 | 0.165 | 73-trc |
| | | | | | Octadecane | | | | | | | |
| A1 | 16.746836 | −88.91311 | 201.73131 | −201.5217 | 75.498293 | | 246.848 | 746.00 | 301.32 | 573.15 | 0.096 | 73-trc |
| | | | | | 7-Hexyltridecane | | | | | | | |
| A2 | 986.90051 | −67.95142 | | | | | | | 310.93 | 408.15 | 0.066 | 59-low/spe |
| | | | | | Eicosane[c] | | | | | | | |
| A1 | 229.21878 | −844.2745 | 1044.9267 | −429.8758 | | | 247.420 | 768.00 | 309.75 | 423.15 | 0.181 | 73-trc |
| A1 | 0.564648 | 3.006777 | −0.800313 | | | | 247.420 | 768.00 | 373.15 | 573.15 | 0.450 | 64-doo |
| | | | | | Docosane | | | | | | | |
| A2 | 984.53036 | −67.26151 | | | | | | | 323.08 | 368.26 | 0.712 | 88-pet/spi[d] |
| | | | | | Tetracosane | | | | | | | |
| A2 | 985.79012 | −64.68799 | | | | | | | 333.52 | 371.22 | 0.279 | 87-pet/van[d] |
| | | | | | 9-Octylheptadecane | | | | | | | |
| A2 | 993.03187 | −65.12813 | | | | | | | 310.93 | 408.15 | 0.036 | 58-cut/mcm, 59-low/spe |
| | | | | | Triacontane | | | | | | | |
| A1 | 0.668899 | 2.176314 | | | | | 249.747 | 857.00 | 373.15 | 573.15 | 0.548 | 64-doo |
| | | | | | 2,6,10,15,19,23-Hexamethyltetracosane | | | | | | | |
| A2 | 991.66650 | −62.70545 | | | | | | | 298.15 | 353.15 | 0.022 | 70-kus/tas |
| | | | | | 11-Decylheneicosane | | | | | | | |
| A2 | 998.52323 | −63.70262 | | | | | | | 310.93 | 408.15 | 0.067 | 59-low/spe |
| | | | | | 13-Dodecylhexacosane | | | | | | | |
| A2 | 1000.9301 | −62.17320 | | | | | | | 310.93 | 408.15 | 0.068 | 59-low/spe |
| | | | | | Tetracontane | | | | | | | |
| A2 | 969.12134 | −46.83596 | −1.614357 | | | | | | 423.15 | 573.15 | 0.062 | 64-doo |
| | | | | | 2-Methyl-1,3-butadiene | | | | | | | |
| A2 | 926.32880 | −66.12200 | −6.000000 | | | | | | 273.15 | 323.15 | 0.000 | 95-trc-2 |
| | | | | | 1-Pentene[e] | | | | | | | |
| A1 | 2.685307 | −6.022579 | 18.874341 | −23.26466 | 10.842690 | | 237.744 | 464.78 | 183.15 | 448.15 | 0.435 | 86-trc-1, 51-day/fel[d] |
| | | | | | 2-Methyl-2-butene | | | | | | | |
| A2 | 865.37793 | −43.70657 | −9.310863 | | | | | | 203.15 | 353.15 | 0.402 | 86-trc-1 |
| | | | | | (*E*)-1,4-Hexadiene | | | | | | | |
| A2 | 993.20963 | −100.020 | | | | | | | 293.15 | 298.15 | 0.000[f] | 75-bur/ric |
| | | | | | (2*Z*,4*E*)-2,4-Hexadiene | | | | | | | |
| A2 | 989.29900 | −92.000 | | | | | | | 293.15 | 298.15 | 0.000[f] | 75-bur/ric |
| | | | | | 1,5-Hexadiene | | | | | | | |
| A2 | 887.62113 | −67.020 | | | | | | | 293.15 | 298.15 | 0.000[f] | 75-bur/ric |
| | | | | | 1-Hexene | | | | | | | |
| A1 | 3.997552 | −14.24428 | 37.259271 | −40.50644 | 16.509841 | | 240.461 | 504.03 | 153.15 | 473.15 | 0.322 | 95-trc |
| | | | | | 1-Heptene[g] | | | | | | | |
| A1 | 4.694761 | −10.48309 | 14.073957 | −5.554842 | | | 243.040 | 537.29 | 223.15 | 523.15 | 0.741 | 95-trc-1, 81-gus/naz[d] |

**Table 6. Continued**

| eq | $a_0$ | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ | $\rho_c$/ kg·m$^{-3}$ | $T_c$/K | $T_{min}$/K | $T_{max}$/K | RMSD/ kg·m$^{-3}$ | ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | 1-Octene | | | | | | |
| A1 | 7.845432 | −20.70510 | 24.728860 | −9.030274 | | | 243.946 | 566.70 | 273.15 | 393.15 | 0.061 | 86-trc |
| | | | | | | 1-Nonene[h] | | | | | | |
| A2 | 960.14191 | −78.76730 | −0.002380 | | | | | | 198.00 | 393.15 | 0.659 | 84-gus/gal, 86-trc |
| | | | | | | 2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene | | | | | | |
| A2 | 1050.7355 | −66.74182 | | | | | | | 298.15 | 353.15 | 0.062 | 70-kus/tas |
| | | | | | | Cyclopentane[i] | | | | | | |
| A1 | 8.142771 | −24.21655 | 31.749720 | −13.20848 | | | 275.037 | 511.70 | 188.63 | 353.15 | 0.174 | 92-bao/cac, 95-trc-3 |
| | | | | | | Methylcyclopentane | | | | | | |
| A1 | 10.138970 | −51.57038 | 121.91233 | −125.5587 | 48.396848 | | 263.829 | 532.73 | 253.15 | 393.15 | 0.081 | 95-trc-3 |
| | | | | | | Cyclohexane | | | | | | |
| A1 | 1.626418 | 0.995043 | −0.255766 | −0.087998 | 0.474534 | | 273.251 | 553.50 | 273.15 | 553.15 | 0.179 | 91-trc |
| | | | | | | Cyclohexane-$d_{12}$ | | | | | | |
| A2 | 1182.0050 | −87.63877 | −3.786667 | | | | | | 288.15 | 313.15 | 0.000[j] | 84-mat/van |
| | | | | | | Methylcyclohexane | | | | | | |
| A1 | 1.626075 | 1.195703 | −0.691798 | 1.908529 | −4.062831 | 2.9225 | 266.816 | 572.20 | 143.15 | 568.15 | 0.168 | 91-trc |
| | | | | | | Cycloheptane | | | | | | |
| A2 | 1062.0709 | −85.68000 | | | | | | | 298.15 | 353.15 | 0.024 | 70-kus/tas |
| | | | | | | Ethylcyclohexane | | | | | | |
| A1 | 4.074781 | −5.478427 | 4.241512 | | | | 269.101 | 602.40 | 263.15 | 383.15 | 0.236 | 92-trc-1 |
| | | | | | | 1-*cis*-2-Dimethylcyclohexane | | | | | | |
| A1 | 2.085256 | −0.339364 | 0.991098 | | | | 269.101 | 601.00 | 263.15 | 343.15 | 0.159 | 91-trc |
| | | | | | | Cyclooctane[k] | | | | | | |
| A1 | 1.258428 | 1.535662 | | | | | 273.696 | 647.20 | 293.15 | 393.85 | 0.314 | 55-kus, 78-gou[d] |
| | | | | | | *trans*-Bicyclo[4.4.0]decane | | | | | | |
| A1 | 1.523238 | 1.203265 | | | | | 280.432 | 687.10 | 298.15 | 353.15 | 0.197 | 70-kus/tas |
| | | | | | | Butylcyclohexane | | | | | | |
| A2 | 1050.0535 | −96.32193 | 3.666554 | | | | | | 253.15 | 393.15 | 0.086 | 92-trc-1 |
| | | | | | | Bicyclohexyl | | | | | | |
| A2 | 1059.0066 | −77.32000 | 5.000000 | | | | | | 298.20 | 338.20 | 0.000[j] | 88-sid/tej |
| | | | | | | Octadecahydrochrysene | | | | | | |
| A2 | 1159.4907 | −61.15625 | | | | | | | 310.93 | 408.15 | 0.081 | 59-low/spe |
| | | | | | | 1,7-Dicyclopentyl-4-(3-cyclopentylpropyl)heptane | | | | | | |
| A2 | 1079.22782 | −64.84824 | | | | | | | 310.95 | 408.15 | 0.147 | 58-cut/mcm |
| | | | | | | 1-(1-Decahydronaphthyl)pentadecane | | | | | | |
| A2 | 1014.2506 | −40.66359 | −3.233775 | | | | | | 333.15 | 408.15 | 0.132 | 58-cut/mcm |
| | | | | | | 1-Cyclopentyl-4-(3-cyclopentylpropyl)dodecane | | | | | | |
| A2 | 1065.4843 | −73.66552 | 1.091535 | | | | | | 310.95 | 408.15 | 0.123 | 58-cut/mcm |
| | | | | | | 1-Cyclohexyl-3-(2-cyclohexylethyl)undecane | | | | | | |
| A2 | 1053.1538 | −63.79427 | | | | | | | 310.95 | 408.15 | 0.122 | 58-cut/mcm |
| | | | | | | 9-(2-Cyclohexylethyl)heptadecane | | | | | | |
| A2 | 1026.5511 | −65.87219 | | | | | | | 310.95 | 408.15 | 0.301 | 58-cut/mcm |
| | | | | | | 9-(3-Cyclopentylpropyl)heptadecane | | | | | | |
| A2 | 1021.2846 | −65.50544 | | | | | | | 310.95 | 408.15 | 0.150 | 58-cut/mcm |
| | | | | | | 1,1-Bis(decahydro-1-naphthyl)undecane | | | | | | |
| A2 | 1111.3631 | −61.42616 | | | | | | | 310.93 | 408.15 | 0.033 | 59-low/spe |
| | | | | | | 1,3-Cyclohexadiene | | | | | | |
| A2 | 1623.1509 | −266.9800 | | | | | | | 293.15 | 298.15 | 0.000[f] | 75-bur/ric |
| | | | | | | 1,4-Cyclohexadiene | | | | | | |
| A2 | 2270.3436 | −482.0200 | | | | | | | 293.15 | 298.15 | 0.000[f] | 75-bur/ric |
| | | | | | | Cyclohexene | | | | | | |
| A1 | 1.328770 | 1.273155 | | | | | 288.028 | 560.48 | 293.15 | 373.15 | 0.073 | 91-mel/mel[d] |

[a] From database 93-cda. Critical densities are given with three decimal points, since they were calculated from rounded values of critical molar volumes recorded in the database 93-cda. [b] Combination of data in temperature ranges: 207.93−298.17 K [93-bao/cac]; 283.15−463.15 K [92-trc]. [c] Average deviation between two fits in the interval 373−423 K is about 1.1 kg·m$^{-3}$. [d] Fit of values obtained by extrapolation along an isotherm of elevated-pressure data to atmospheric or saturation pressure ($P_{ref}$) using the Tait equation. [e] Combination of data in temperature ranges: 183.15−323.15 K [86-trc-1]; 353.15−448.15 K [51-day/fel]. [f] Two density values available. [g] Combination of data in temperature ranges: 223.15−363.15 K [95-trc-1]; 373.15−523.15 K [81-gus/naz]. [h] Combination of data in temperature ranges: 198.00−248.00 K [84-gus/gal]; 273.15−393.15 K [86-trc]. [i] Combination of data in temperature ranges: 188.63−302.08 K [92-bao/cac]; 263.15−353.15 K [95-trc-3]. [j] Polynomial interpolation. [k] Combination of data in temperature ranges: 293.15−353.15 K [55-kus]; 373.75−393.85 K [78-gou].

selected to get the correct derivative of the liquid−vapor saturation line at the critical point, $(d\rho/dT) \rightarrow -\infty$ for $T \rightarrow T_c$.

In the cases of the $P-\rho-T$ data sets for 1-octene and cyclohexane (denoted by the letter e in the last column of Table 4) where the reference density values $\rho(T,P_{ref}(T))$ (see

eq 1) were not available (nor original values, nor extrapolated ones), the reference density values calculated from the fits presented in Table 6 were employed in fitting the $P-\rho-T$ data by the Tait equation. The fits for other substances are presented in Table 6 as auxiliary information here, which may be useful particularly for less common substances. The functions can be used to calculate smoothed reference density values for evaluation of compressed liquid densities $\rho(T,P)$ from eq 1. Except for the fits of the values taken from the TRC Tables, the fits in Table 6 do not represent critically selected experimental data.

The densities [92-trc] for 2,3-dimethylbutane at low temperatures do not agree with the data of Baonza et al. [93-bao/cac] and Riembauer et al. [90-rie/sch]. Besides that, the fit of the values of the TRC Tables [92-trc] required seven parameters in eq A1 to get a satisfactory result. Replacement of the low-to-ambient-temperature densities [92-trc] by the values reported by Baonza et al. [93-bao/cac] led to the fit with four parameters. Two fits are presented in Table 6 for eicosane; the deviations of the first fit from the second one in the overlapping temperature range are rather large (from $-1.1$ kg·m$^{-3}$ to 2.6 kg·m$^{-3}$). The densities of 1-heptene at saturation pressure [83-mcg] obtained by the extrapolation of data [81-gus/naz] are consistent with the values of the TRC Tables [95-trc-1]; the fit of the combined data in Table 6 exhibits, however, the point of inflection at $T = 517$ K. The fit for cyclopentane does not cover the entire range of data [95-trc-3], since large deviations were observed for $T > 363$ K (up to the highest temperature 393.15 K); the fit could be improved by enlargement of the number of parameters in eq A1, but the fits with $a_0 < 0$ and two points of inflection resulted. Extrapolated values [78-gou] for cycloheptane are by about 1.5 kg·m$^{-3}$ lower than the direct data of Kuss and Taslimi [70-kus/tas]; therefore, the two data sets were not combined for the fit. The data for cyclooctane from the same laboratory [55-kus] were combined with extrapolated values [78-gou] for $T \geq 373.15$ K; the values for lower temperatures were rejected, since they differ from the data of Kuss [55-kus] by $-1.5$ kg·m$^{-3}$.

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