International Journal of Thermophysics, Vol. 24, No. 5, September 2003 (© 2003)

Thermodynamic Properties of Heavy *n*-Alkanes in the Liquid State: *n*-Dodecane[1]

T. S. Khasanshin,[2,3] A. P. Shchamialiou,[2] and O. G. Poddubskij[2]

A grid algorithm based on sound speed data, was used to calculate the thermodynamic properties of liquid *n*-dodecane. The density, isobaric expansion coefficient, isothermal compressibility, isobaric and isochoric heat capacities, enthalpy, and entropy of liquid *n*-dodecane were calculated in the range of temperatures from 293 to 433 K and pressures from 0.1 to 140 MPa. Coefficients of the Tait equation were determined in the above-identified range of parameters. A table of the thermodynamic properties of *n*-dodecane is presented.

KEY WORDS: density; enthalpy; entropy; heat capacity; isobaric expansion coefficient; isothermal compressibility; *n*-dodecane; sound velocity.

1. INTRODUCTION

This study is a continuation of studies [1–4] which deal with the thermodynamic properties of higher *n*-alkanes in the liquid phase. Information on the thermodynamic properties of alkanes is available only for light homologues. Heavy homologues have been investigated to a smaller degree, and their properties need to be refined. The acoustic method was used to obtain desired information about the properties of alkanes. In using this method, one must have as input experimental results for the dependences of density and isobaric heat capacity on temperature at atmospheric pressure and of sound speed on temperature and pressure.

In this study, we calculated the thermodynamic properties of liquid *n*-dodecane at temperatures from 293 to 433 K and at pressures up to 140 MPa.

---

[1] Paper presented at the Sixteenth European Conference on Thermophysical Properties, September 1–4, 2002, London, United Kingdom.

[2] Mogilev State University of Foodstuffs, Shmidt av. 3, 212027 Mogilev, Belarus.

[3] To whom correspondence should be addressed. E-mail: khasanshin@tut.by

2. INPUT DATA

As input data for the sound speed, we used the results of our measurements [1] performed using the pulse-echo overlap method at temperatures of 303 to 433K and pressures up to 50 MPa with an uncertainty of 0.1%, data [5] at atmospheric pressure and temperatures 293 to 373 K, data [6] at temperatures 273 to 473 K and pressures 0.1 to 140 MPa, data [7] at the temperature 298.15 K and pressures 0.1 to 100 MPa, data [8] at temperatures 303 to 393 K and pressures 0.1 to 196.2 MPa, and data [9] at temperatures 303 to 433 K and pressures 0.1 to 608.9 MPa. The measurements reported in Refs. 6 and 7 were performed with uncertainties of 0.1%, and the measurements in Refs. 5, 8, and 9 were performed with uncertainties of 0.05, 0.2, and 0.3%, respectively. Analysis of the initial data has revealed mutual agreement of the results reported in Refs. 1, 5, and 6, with deviations not exceeding 0.1%. The measurements reported in Ref. 7 are higher by 0.2 to 0.3% on average, and those in Refs. 8 and 9 are lower by 0.2 to 0.3% on average than the set of mutually agreeing data of Refs. 1, 5, and 6.

The resulting set of data from Refs. 1 and 5–9 for the sound speed at $T = 293$ to 433 K and $P = 0.1$ to 140 MPa was represented as a function of temperature and pressure by

$$u = \sum_{i=0}^{4} \sum_{j=0}^{6} a_{ij} (T/1000)^i \, (P/100)^j, \tag{1}$$

where u is the sound speed in $\mathrm{m \cdot s^{-1}}$, T is the temperature in K, and P is the pressure in MPa. The values of the regressed coefficients a_{ij} are given in Table I.

Table I. Coefficients a_{ij} of Eq. (1)

	i				
j	0	1	2	3	4
0	2.192471907×10^3	-4.555955037×10^2	-1.690361673×10^4	3.374553628×10^4	-2.150705438×10^4
1	-2.684469556×10^3	4.286646490×10^4	-2.140437206×10^5	4.658137747×10^5	-3.543532428×10^5
2	7.487338276×10^3	-1.173846131×10^5	6.141682773×10^5	-1.329013880×10^6	9.904812512×10^5
3	8.295510847×10^3	-3.617570056×10^4	-5.021640246×10^4	3.624489695×10^5	-3.111887465×10^5
4	-2.891310112×10^4	2.660937618×10^5	-9.243185428×10^5	1.508679039×10^6	-1.054478107×10^6
5	2.247132466×10^4	-2.168341482×10^5	8.016039340×10^5	-1.392521300×10^6	9.953796339×10^5
6	-5.725095051×10^3	5.480309126×10^4	-2.018509988×10^5	3.508868252×10^5	-2.508361360×10^5

At atmospheric pressure, the temperature dependences of density ρ_0 from Ref. 10 are used. For the heat capacity c_p there are data only in a narrow range of temperatures 267 to 317 K, which do not cover the calculated interval of temperatures 293 to 433 K. To obtain the dependence $c_{p0} = f(T)$ at atmospheric pressure, which is necessary for the calculation of the thermodynamic properties at high pressure, the behavior of the heat capacity in the homologous *n*-alkane series having the common formula C_nH_{2n+2} was investigated. For this purpose, the results of the generalization of the heat capacity for separate homologues from C_5 up to C_{18} were used in an interval of temperatures 273 to 433 K recommended in a review [11]. At atmospheric pressure and constant temperatures these was observed a smooth change (almost linear) of the molar isobaric heat capacity within the limits of uncertainty of the recommended values (0.25 to 1%) depending on the number of carbon atoms in the homologues. This was used to obtain the values of heat capacity for C_{12} at temperatures 293 to 433 K by interpolation of the molar heat capacity using the dependence on the number of carbon atoms in an *n*-alkane. These heat capacity values, as well as those of the density reported in the paper [10], were represented as a temperature-dependent function in the form,

$$\rho_0 = 929.1654 - 0.5174730T - 3.338672 \times 10^{-4}T^2, \tag{2}$$

$$\begin{aligned} c_{p0} = {} & 2.273845 - 4.559779 \times 10^{-3}T \\ & + 1.843537 \times 10^{-5}T^2 - 1.306521^{-8}T^3, \end{aligned} \tag{3}$$

where ρ_0 is the density in $\mathrm{kg \cdot m^{-3}}$ and c_{p0} is the isobaric heat capacity in $\mathrm{kJ \cdot kg^{-1} \cdot K^{-1}}$ at atmospheric pressure. Equations (2) and (3) reproduce values of ρ_0 and c_{p0} with deviations less than the estimated uncertainty.

We estimated that the error of the input data used to calculate the thermodynamic properties does not exceed 0.1% with respect to ρ_0 and u and 1% with respect to c_{p0}.

3. CALCULATION METHOD

The procedure for the calculation of the thermodynamic properties is based on the following known thermodynamic relations:

$$\left(\frac{\partial \rho}{\partial P}\right)_T = \frac{1}{u^2} + \frac{T\alpha^2}{c_p}, \tag{4}$$

$$\left(\frac{\partial c_p}{\partial P}\right)_T = -\frac{T}{\rho}\left[\alpha^2 + \left(\frac{\partial \alpha}{\partial T}\right)_P\right]. \tag{5}$$

Here ρ is the density, c_p is the specific heat capacity at constant pressure, and α is the thermal expansion defined by $\alpha = -(\partial\rho/\partial T)_p/\rho$. For simplifying numerical solutions, Eqs. (4) and (5) can be written in a dimensionless form using the dimensionless pressure π, dimensionless temperature τ, dimensionless density D, dimensionless sound velocity U as it was offered by Kiselev et al. [12], and dimensionless variables n and m, defined by

$$\pi = (p - p_0)/p_0, \tag{6}$$

$$\tau = (T - T_0)/T_0, \tag{7}$$

$$D = \rho R T_0/p_0; \tag{8}$$

$$U = RT_0/u^2, \tag{9}$$

$$n = \frac{c_p}{R(\tau+1)}, \tag{10}$$

$$m = \left(\frac{\partial}{\partial\tau}\frac{1}{D}\right)_\pi, \tag{11}$$

where T_0 and p_0 are the temperature and pressure of some standard system.

Thus, we have obtained the following set of equations in a dimensionless form

$$\left(\frac{\partial D}{\partial\pi}\right)_\tau = U + \frac{D^2 m^2}{n}, \tag{12}$$

$$\left(\frac{\partial n}{\partial\pi}\right)_\tau = -\left(\frac{\partial m}{\partial\tau}\right)_\pi, \tag{13}$$

$$\left(\frac{\partial}{\partial\tau}\frac{1}{D}\right)_\pi = m. \tag{14}$$

The set of Eqs. (12) to (14) can be solved numerically using a grid algorithm in a rectangle $0 \leqslant \pi \leqslant \pi_{\max}$, $0 \leqslant \tau \leqslant \tau_{\max}$ with the known initial conditions $D(\pi = 0, \tau)$, $n(\pi = 0, \tau)$, and $m(\pi = 0, \tau)$ and set of dimensionless sound velocities $U(\pi, \tau)$ in the entire rectangle.

The initial conditions $D(0, \tau)$ and $n(0, \tau)$ were defined by Eqs. (8) and (10) from the data on the density ρ_0 and isobaric heat capacity c_{p0} at atmospheric pressure, which are given by Eqs. (2) and (3). The initial condition $m(0, \tau)$ was obtained from the initial condition $D(0, \tau)$ by using Eq. (11). The set of the sound velocity $U(\pi, \tau)$ was obtained from Eqs. (1) and (9). It was assumed that $T_0 = 293.15$ K and $p_0 = 0.1$ MPa.

The set of Eqs. (12) to (14) was solved by the finite-difference method and a pressure-temperature grid was employed with a small temperature grid size $\Delta\tau$ and pressure grid size $\Delta\pi$. The values of dimensionless temperature for a row i were determined from $\tau_i = i\,\Delta\tau$, $i = 0, 1, 2, \ldots, I$ and the values of dimensionless pressure for a row j were determined from $\pi_j = j\,\Delta\pi$, $j = 0, 1, 2, \ldots, J$, where I and J are total numbers of points per row.

We have employed a grid with the right-hand derivatives. In this case the Eqs. (12) to (14) have been written in the form,

$$D_{i,j+1} = D_{i,j} + U_{i,j}\,\Delta\pi + \frac{D_{i,j}^2 \bar{m}_{i,j}^2}{n_{i,j}}\,\Delta\pi, \qquad [i \in (0, I-j)] \tag{15}$$

$$m_{i,j} = \left(\frac{1}{D_{i+1,j}} - \frac{1}{D_{i,j}}\right)\frac{1}{\Delta\tau}, \qquad [i \in (0, I-j)] \tag{16}$$

$$\bar{m}_{i,j} = \sum_{l=-K}^{K} m_{i+l,j} \cdot \frac{1}{2K+1}, \qquad [i \in (0, I-j)] \tag{17}$$

$$n_{i,j+1} = n_{i,j} + (\bar{m}_{i,j} - \bar{m}_{i+1,j})\,\frac{\Delta\pi}{\Delta\tau}, \qquad [i \in (0, I-j-1)]. \tag{18}$$

Here, $\bar{m}_{i,j}$ is the average value of $m_{i,j}$ for $2K+1$ points.

One can see that the number of grid points per τ decreases by unity on the right with every next row j; i.e., the solution is actually obtained on a triangular grid. In order to obtain a solution on the rectangular grid, we employed a similar independent triangular grid with the left-hand derivatives, for which the number of grid points per τ decreases by unity on the left with every next row j. In this case Eqs. (12) to (14) have been written in the form,

$$D_{i,j+1} = D_{i,j} + U_{i,j}\,\Delta\pi + \frac{D_{i,j}^2 \bar{m}_{i,j}^2}{n_{i,j}}\,\Delta\pi, \qquad [i \in (j, I)] \tag{19}$$

$$m_{i,j} = \left(\frac{1}{D_{i,j}} - \frac{1}{D_{i-1,j}}\right)\frac{1}{\Delta\tau}, \qquad [i \in (j, I)] \tag{20}$$

$$\bar{m}_{i,j} = \sum_{l=-K}^{K} m_{i+l,j} \cdot \frac{1}{2K+1}, \qquad [i \in (j, I)] \tag{21}$$

$$n_{i,j+1} = n_{i,j} + (\bar{m}_{i-1,j} - \bar{m}_{i,j})\,\frac{\Delta\pi}{\Delta\tau}, \qquad [i \in (j+1, I)]. \tag{22}$$

We supplemented the points calculated on the grid with the right-hand derivatives with the points calculated on the grid with the left-hand derivatives to obtain an algorithm on the rectangular grid.

The calculation of the values $D_{i,j+1}$ and $n_{i,j+1}$ from Eqs. (15), (19) and (18), (22) at $\pi_{j+1}=\pi_j+\Delta\pi$ were started from $j=0$ ($p=0.1$ MPa), at which the quantities $D_{i,j}$, $n_{i,j}$, and $m_{i,j}$ are obtained by using Eqs. (2), (8), (3), (10), and (11). Then the number of row j was increased by unity ($j=j+1$) and values of $m_{i,j}$ and $\bar{m}_{i,j}$ were computed by using Eqs. (16), (20) and (17), (21) and values of $D_{i,j+1}$ and $n_{i,j+1}$ were computed from Eqs. (15), (19) and (18), (22) at the next pressure $\pi_{j+1}=\pi_j+\Delta\pi$. These operations were repeated until the row number reaches J and the pressure reaches a maximum at which the sound speed is still known.

The density ρ, isobaric expansion coefficient α, and isobaric heat capacity c_p were calculated from Eqs. (8), (11), and (10), using the obtained sets of the values of D_{ij}, $\bar{m}_{i,j}$, and n_{ij}. Further, we used obtained values of ρ, α, c_p, and u to calculate the isothermal compressibility β_T, isochoric heat capacity c_v, enthalpy h, and entropy s by applying the following thermodynamic relations:

$$\beta_T=\frac{1}{\rho}\left(\frac{1}{u^2}+\frac{T\alpha^2}{c_p}\right), \tag{23}$$

$$c_v=\frac{c_p}{(1+\frac{T\alpha^2u^2}{c_p})}, \tag{24}$$

$$h=h_0+\int_{T_0}^{T} c_{p0}\, dT+\int_{p_0}^{p}\frac{1}{\rho}(1-T\alpha)\, dp, \tag{25}$$

$$s=s_0+\int_{T_0}^{T}\frac{c_{p0}}{T}\, dT-\int_{p_0}^{p}\frac{\alpha}{\rho}\, dp. \tag{26}$$

In order to calculate the thermodynamic properties with an acceptable accuracy, we chose a temperature grid size $\Delta\tau=8.9\times10^{-4}$ ($\Delta T=0.26$ K) and a pressure grid size $\Delta\pi=0.56$ ($\Delta P=0.056$ MPa). We assumed that $h_0=0$ and $s_0=0$ at $T_0=293.15$ K and $P_0=0.1$ MPa.

We estimate uncertainties of the calculated values at atmospheric pressure is less than 0.1% for ρ, 0.25 to 1% for c_p, 0.7 to 1.5% for c_v, 1% for α, and 0.7% for β_T; and at $p=140$ MPa and $T=433$ K, 0.2% for ρ, 1.8% for c_p, 2.5% for c_v, 2.3% for α, and 1% for β_T.

The calculation procedure was described in detail in Ref. 2. The calculated results are given in Tables II–IX.

Table II. Speed of Sound u ($\mathrm{m \cdot s^{-1}}$) in *n*-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	1298.2	1222.3	1148.1	1076.0	1006.0	938.4	873.1	810.1
5	1327.1	1253.1	1181.4	1112.2	1045.6	981.7	920.4	861.4
10	1355.2	1283.1	1213.6	1146.9	1083.3	1022.5	964.4	908.5
20	1407.8	1339.0	1273.2	1210.7	1151.5	1095.5	1042.1	990.9
30	1456.1	1390.2	1327.5	1268.3	1212.4	1159.8	1109.8	1061.9
40	1500.9	1437.5	1377.5	1321.0	1267.8	1217.7	1170.3	1124.9
50	1542.9	1481.7	1424.0	1369.7	1318.8	1270.8	1225.4	1182.2
60	1582.5	1523.3	1467.6	1415.4	1366.3	1320.1	1276.4	1234.8
70	1620.2	1562.7	1508.9	1458.4	1410.9	1366.2	1323.9	1283.5
80	1656.3	1600.3	1548.0	1499.1	1453.0	1409.6	1368.3	1328.9
90	1691.0	1636.4	1585.4	1537.7	1492.9	1450.5	1410.2	1371.5
100	1724.7	1671.0	1621.0	1574.3	1530.6	1489.2	1449.9	1411.9
120	1788.3	1736.2	1687.8	1642.7	1600.6	1561.2	1524.0	1488.4
140	1844.4	1796.2	1750.3	1706.9	1666.0	1627.6	1591.7	1558.2

Table III. Density ρ ($\mathrm{kg \cdot m^{-3}}$) of *n*-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	748.8	734.4	719.7	704.8	689.6	674.1	658.4	642.4
5	752.2	738.2	724.0	709.7	695.1	680.4	665.5	650.5
10	755.5	741.9	728.2	714.3	700.3	686.2	672.1	657.9
20	761.8	748.9	735.9	722.8	709.8	696.7	683.6	670.7
30	767.6	755.2	742.9	730.5	718.1	705.8	693.6	681.6
40	773.0	761.1	749.3	737.5	725.7	714.0	702.5	691.1
50	778.1	766.7	755.3	743.9	732.7	721.5	710.4	699.6
60	782.9	771.8	760.9	749.9	739.1	728.3	717.7	707.4
70	787.4	776.7	766.1	755.5	745.0	734.7	724.5	714.5
80	791.8	781.4	771.1	760.8	750.7	740.6	730.7	721.1
90	795.9	785.8	775.8	765.8	755.9	746.2	736.6	727.3
100	799.9	790.0	780.3	770.5	760.9	751.5	742.1	733.0
120	807.3	798.0	788.6	779.4	770.3	761.2	752.4	743.7
140	814.3	805.3	796.4	787.5	778.8	770.1	761.6	753.3

Table IV. Isobaric Heat Capacity c_p ($kJ \cdot kg^{-1} \cdot K^{-1}$) of *n*-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	2.192	2.253	2.318	2.387	2.460	2.537	2.615	2.696
5	2.187	2.247	2.311	2.380	2.452	2.527	2.605	2.684
10	2.183	2.242	2.306	2.374	2.445	2.520	2.594	2.669
20	2.175	2.234	2.297	2.364	2.435	2.509	2.583	2.657
30	2.169	2.227	2.289	2.356	2.427	2.501	2.575	2.649
40	2.164	2.221	2.283	2.350	2.421	2.495	2.570	2.644
50	2.160	2.217	2.279	2.345	2.416	2.491	2.566	2.641
60	2.156	2.213	2.275	2.341	2.412	2.487	2.563	2.638
70	2.153	2.209	2.271	2.338	2.409	2.485	2.561	2.637
80	2.150	2.207	2.268	2.335	2.406	2.482	2.559	2.636
90	2.147	2.204	2.265	2.332	2.403	2.481	2.558	2.635
100	2.145	2.201	2.263	2.330	2.401	2.479	2.557	2.634
120	2.141	2.197	2.259	2.326	2.398	2.477	2.556	2.634
140	2.138	2.194	2.255	2.322	2.395	2.475	2.555	2.634

Table V. Isobaric Expansion Coefficient $\alpha \times 10^3$ (K^{-1}) of *n*-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	0.953	0.990	1.028	1.069	1.112	1.157	1.205	1.256
5	0.922	0.954	0.986	1.019	1.053	1.087	1.122	1.155
10	0.894	0.921	0.948	0.976	1.003	1.029	1.054	1.075
20	0.844	0.865	0.885	0.904	0.922	0.938	0.951	0.958
30	0.802	0.818	0.833	0.847	0.859	0.869	0.875	0.875
40	0.766	0.778	0.790	0.800	0.809	0.815	0.817	0.813
50	0.734	0.744	0.753	0.760	0.767	0.770	0.770	0.763
60	0.705	0.713	0.720	0.726	0.731	0.733	0.731	0.723
70	0.680	0.686	0.692	0.697	0.700	0.701	0.698	0.689
80	0.657	0.662	0.667	0.671	0.673	0.673	0.669	0.660
90	0.636	0.641	0.644	0.647	0.649	0.648	0.644	0.634
100	0.617	0.621	0.624	0.626	0.627	0.626	0.621	0.612
120	0.583	0.586	0.588	0.590	0.590	0.588	0.583	0.574
140	0.553	0.556	0.557	0.558	0.558	0.557	0.552	0.544

Table VI. Isothermal Compressibility $\beta_T \times 10^3$ (MPa^{-1}) of *n*-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	0.955	1.097	1.265	1.465	1.705	1.993	2.341	2.766
5	0.906	1.034	1.183	1.356	1.559	1.795	2.074	2.403
10	0.863	0.978	1.111	1.263	1.436	1.635	1.863	2.126
20	0.788	0.885	0.993	1.113	1.246	1.394	1.558	1.741
30	0.728	0.810	0.900	0.998	1.105	1.222	1.348	1.484
40	0.677	0.748	0.825	0.908	0.996	1.091	1.192	1.299
50	0.634	0.696	0.763	0.834	0.909	0.988	1.072	1.159
60	0.596	0.652	0.710	0.772	0.837	0.904	0.975	1.048
70	0.564	0.613	0.665	0.719	0.776	0.835	0.896	0.958
80	0.535	0.579	0.626	0.674	0.724	0.776	0.830	0.884
90	0.509	0.549	0.592	0.635	0.680	0.726	0.773	0.821
100	0.485	0.523	0.561	0.601	0.641	0.683	0.725	0.767
120	0.445	0.477	0.510	0.543	0.577	0.611	0.645	0.679
140	0.413	0.440	0.467	0.496	0.525	0.554	0.583	0.610

Table VII. Isochoric Heat Capacity c_v (kJ $\cdot$ kg^{-1} $\cdot$ K^{-1}) of *n*-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	1.820	1.872	1.931	1.997	2.068	2.145	2.226	2.311
5	1.822	1.874	1.933	1.999	2.070	2.147	2.228	2.314
10	1.824	1.876	1.935	2.001	2.072	2.149	2.230	2.317
20	1.828	1.880	1.939	2.005	2.076	2.152	2.235	2.324
30	1.832	1.884	1.943	2.009	2.079	2.156	2.240	2.332
40	1.836	1.888	1.947	2.012	2.083	2.160	2.244	2.339
50	1.840	1.892	1.951	2.016	2.086	2.163	2.249	2.345
60	1.844	1.896	1.955	2.019	2.090	2.167	2.253	2.351
70	1.848	1.900	1.958	2.022	2.092	2.170	2.257	2.357
80	1.851	1.903	1.961	2.025	2.095	2.173	2.261	2.363
90	1.855	1.906	1.964	2.028	2.098	2.176	2.264	2.368
100	1.858	1.909	1.967	2.030	2.101	2.179	2.268	2.373
120	1.864	1.915	1.972	2.036	2.106	2.185	2.275	2.382
140	1.871	1.921	1.977	2.040	2.111	2.189	2.281	2.391

Table VIII. Enthalpy h ($\mathrm{kJ \cdot kg^{-1}}$) of n-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	0.0	44.4	90.1	137.2	185.6	235.6	287.1	340.2
5	4.7	49.1	94.6	141.5	189.8	239.6	290.9	343.8
10	9.6	53.8	99.3	146.1	194.3	243.9	295.0	347.8
20	19.4	63.5	108.8	155.4	203.4	252.8	303.7	356.2
30	29.4	73.3	118.4	164.9	212.7	262.0	312.8	365.1
40	39.4	83.2	128.2	174.6	222.3	271.4	322.1	374.4
50	49.4	93.2	138.1	184.3	231.9	281.0	331.6	383.9
60	59.5	103.2	148.1	194.2	241.7	290.7	341.3	393.5
70	69.7	113.3	158.1	204.2	251.6	300.5	351.0	403.3
80	79.9	123.4	168.1	214.2	261.6	310.4	360.9	413.1
90	90.1	133.6	178.2	224.2	271.6	320.4	370.8	423.1
100	100.3	143.8	188.4	234.3	281.6	330.4	380.8	433.1
120	120.8	164.2	208.7	254.6	301.8	350.5	400.9	453.2
140	141.4	184.7	229.2	274.9	322.1	370.8	421.2	473.5

Table IX. Entropy s ($\mathrm{kJ \cdot kg^{-1} \cdot K^{-1}}$) of n-Dodecane

	T (K)							
P (MPa)	293.15	313.15	333.15	353.15	373.15	393.15	413.15	433.15
0.1	0.0	0.1467	0.2881	0.4253	0.5588	0.6892	0.8170	0.9426
5	−0.0061	0.1402	0.2813	0.4180	0.5511	0.6811	0.8084	0.9335
10	−0.0121	0.1339	0.2746	0.4110	0.5438	0.6734	0.8003	0.9250
20	−0.0236	0.1219	0.2621	0.3980	0.5301	0.6592	0.7856	0.9097
30	−0.0343	0.1107	0.2505	0.3859	0.5177	0.6463	0.7724	0.8962
40	−0.0445	0.1002	0.2397	0.3747	0.5061	0.6345	0.7602	0.8839
50	−0.0542	0.0902	0.2294	0.3642	0.4953	0.6234	0.7490	0.8726
60	−0.0634	0.0808	0.2197	0.3543	0.4852	0.6131	0.7385	0.8620
70	−0.0722	0.0717	0.2105	0.3448	0.4755	0.6033	0.7286	0.8521
80	−0.0807	0.0631	0.2016	0.3358	0.4664	0.5940	0.7192	0.8427
90	−0.0888	0.0548	0.1931	0.3272	0.4576	0.5851	0.7103	0.8338
100	−0.0967	0.0468	0.1850	0.3189	0.4492	0.5766	0.7017	0.8253
120	−0.1116	0.0316	0.1695	0.3032	0.4333	0.5606	0.6856	0.8092
140	−0.1256	0.0174	0.1551	0.2885	0.4185	0.5456	0.6706	0.7943

4. DISCUSSION OF RESULTS

The density of *n*-dodecane was measured by Boelhouwer [13] in the temperature range from 303 to 393 K and at pressures up to 117.8 MPa, Cutler et al. [14] measured the density of *n*-dodecane at temperatures from 311 to 408 K and at pressures up to 689 MPa, Landau and Würflinger [15] reported density data obtained in the range from 268.45 to 313 K at pressures of 10 to 240 MPa, Dymond et al. [16] measured the density in the range of temperatures from 298 to 373 K and at pressures from 0.1 to 441.9 MPa with an uncertainty of 0.1 to 0.2%, and Tanaka et al. [17] also reported results of measurements performed at temperatures from 298 to 348 K and at pressures up to 150.8 MPa with an uncertainty of 0.1%. There are also results of generalizations reported by Assael et al. [18] and by Cibulka and Hnědkovský [19] in the range of temperatures from 268 to 393 K and from 298 to 393 K and pressures from 0.1 to 441.9 and 0.1 to 420 MPa, respectively. Assael et al. [18] used a Tait equation to correlate densities of *n*-alkanes. The correlation covers the *n*-alkanes from methane (C_1) to *n*-hexadecane (C_{16}) in an extended pressure range up to 500 MPa in some cases. The overall average deviation of the experimental measurements of the density from those calculated by the correlation is $\pm 0.10\%$.

Comparison between our calculated values of density and measured data reported in Refs. 13 and 15–17 as well as smoothed density values reveals agreement within 0.1 to 0.3%. A significant deviation (1% on average) is found with the data reported in Ref. 14. A comparison of isothermal compressibility values obtained by us with those calculated by Boelhouwer [13] who used *PvT* data at temperatures from 303 to 393 K and pressures from 0.1 to 117.8 MPa revealed that the values of β_T from Ref. 13 are lower on average by 2.5%. However, this does not exceed the total uncertainty of calculations. To facilitate the calculation of density ρ, we generalized the obtained values with the Tait equation,

$$\rho = \rho_0 / (1 - A \ln[(B + P)/(B + P_0)]), \tag{27}$$

where A is a constant and B is a function depending on temperature,

$$B = \sum_{i=0}^{2} b_i (T_c/T)^i. \tag{28}$$

Here, T_c is the critical temperature, $T_c = 658.6$ K [18]. The coefficients of Eqs. (27) and (28) are given below,

$$A = 0.0881; \qquad b_0 = -77.51; \qquad b_1 = 63.67; \qquad b_2 = 5.639.$$

Equation (27) describes well the calculated values of density in the investigated range of parameters: $T = 293$ to 433 K and $P = 0.1$ to 140 MPa. The standard and maximum deviations of density ρ calculated by Eq. (27) from the calculated values do not exceed 0.01 and 0.04%, respectively. It should be noted that Eq. (27) has good extrapolation capabilities depending on pressure. This is demonstrated by the reproduction with sufficient accuracy (0.1 to 0.3%) at pressures up to 400 MPa of values of density given in Refs. 15–19 at pressures up to 400 MPa. Thus, it may be assumed that the values of density, calculated by Eq. (27), for temperatures 393 to 433 K and pressures from 140 to 400 MPa (the range of parameters that has not been systematically investigated previously) will have an uncertainty of 0.1 to 0.3%, or less.

5. CONCLUSION

Equation (27) may be recommended for practical calculations at pressures from 0.1 to 400 MPa and at temperatures from 293 to 433 K. The calculations and comparisons give evidence of the reliability of the proposed calculation method and of the obtained results.

REFERENCES

1. T. S. Khasanshin and A. P. Shchemelev, *High Temp.* **39**:60 (2001). Translated from *Teplofiz. Vys. Temp.* **39**:64 (2001).
2. D. V. Dovnar, Yu. A. Lebedinskii, T. S. Khasanshin, and A. P. Shchemelev, *High Temp.* **39**:835 (2001). Translated from *Teplofiz. Vys. Temp.* **39**:899 (2001).
3. T. S. Khasanshin and A. P. Shchemelev, *High Temp.* **40**:207 (2002). Translated from *Teplofiz. Vys. Temp.* **40**:235 (2002).
4. T. S. Khasanshin and A. P. Shchamialiov, *High Temp.-High Press.* **32**:663 (2000).
5. F. Plantier, J. L. Daridon, B. Lagourette, and C. Boned, *High Temp.-High Press.* **32**:305 (2000).
6. J. W. M. Boelhouwer, *Physica* **34**:484 (1967).
7. T. Takagi and H. Teranishi, *Fluid Phase Equilib.* **20**:315 (1985).
8. B. S. Kiriakov and N. F. Otpushchennikov, *Nauch. Tr. Kursk. Gos. Ped. Inst.* **7**:16 (1972).
9. Yu. F. Melikhov, *Acoustic Researches of Equilibrium Properties and Equations of State of Multinuclear Liquids at High Pressures Cand. Sci. (Phys.-Math.) Dissertation*, Vol. 2 (Kursk State Ped. Inst., Kursk, 1984), pp. 227–228.
10. I. Cibulka, *Fluid Phase Equilib.* **89**:1 (1993).
11. V. Růžička, M. Zábranský, and V. Majer, *J. Phys. Chem. Ref. Data* **20**:405 (1991).
12. O. E. Kiselev, D. A. Tikhonov, G. N. Sarkisov, and A. P. Sarvazyan, *Dokl. Ross. Akad. Nauk.* **331**:302 (1993).
13. J. W. M. Boelhouwer, *Physica* **26**:1021 (1960).
14. W. G. Cutler, R. H. McMickle, W. Webb, and R. W. Schiessler, *J. Chem. Phys.* **29**:727 (1958).

15. R. Landau and A. Würflinger, *Ber. Bunsen. Phys. Chem.* **84**:895 (1980).
16. J. H. Dymond, J. Robertson, and J. D. Isdale, *J. Chem. Thermodyn.* **14**:51 (1982).
17. Y. Tanaka, H. Hosokawa, and T. Makita, *Int. J. Thermophys.* **12**:245 (1991).
18. M. J. Assael, J. H. Dymond, and D. Exadaktilou, *Int. J. Thermophys.* **15**:155 (1994).
19. I. Cibulka and L. Hnědkovský, *J. Chem. Eng. Data* **41**:657 (1996).