Speeds of Sound, Densities, and Isentropic Compressibilities of 1-Chlorohexane at Temperatures from (293.15 to 413.15) K and Pressures up to 200 MPa

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Experimental speeds of sound and densities are presented for the liquid phase of 1-chlorohexane. The measurements were carried out along seven isotherms from (293.15 to 413.15) K at pressures from saturation up to 200 MPa. The speed of sound was measured by a pulse-phase echo ultrasonic device at a frequency of (1 and 5) MHz with an uncertainty of ± 0.2 %. The density was measured by an acoustic piezometer with an uncertainty of ± 0.3 %. The experimental results have been used to calculate isentropic compressibility (k_S) with an uncertainty of ± 1 %. The temperature and pressure variation of sound speed, density, and isentropic compressibility are discussed. The experimental results were used to calculate various thermophysical properties such as isobaric thermal expansion coefficient (α_P), isothermal compressibility (k_T), temperature coefficient of pressure at constant volume ($(\partial P/\partial T)_V$), and internal pressure (P_i).

Introduction

The knowledge of thermophysical properties of organic liquids at high temperatures and pressures is the particular importance for chemical technology. In recent years the interest to measurement of the sound speed in organic liquids has considerably increased.[1,2] In contrast to the *n*-alkanes, which have been studied by acoustic method in single-phase area,[3−8] acoustic properties of their halogen-substituted analogues are less well understood.[9] This could relate to the high chemical activity and relative thermal instability of certain haloalkanes. Presently, the sphere of application of haloalkanes is wide, including raw material for synthesis of alkanes and alkenes, solvents, anesthetics, insecticides, bactericidal preparations, etc.

In our earlier work,[10] we studied the speed of sound and density of 1-chlorohexane along the saturation line from (293.15 to 373.15) K. To the best of our knowledge, the speed of sound and density of 1-chlorohexane at high pressures has not been studied. For this reason, we present here new experimental data of the speed of sound and density for the 1-chlorohexane in the range of temperature from (293.15 to 413.15) K at high pressure from saturation up to 200 MPa. These data are of interest because of the effect on the molecular interactions of chlorine substitution in *n*-alkanes.

Experimental Section

1-Chlorohexane used in this study (mole fraction > 0.99) was supplied by Sigma-Aldrich Ltd. and was used without further purification. The ultrasonic speed was measured using a pulse-phase echo ultrasonic device[11] with an uncertainty of ± 0.2 % at a frequency of (1 and 5) MHz. Dispersion was not observed. All experimental data were conducted along seven isotherms spaced at 20 K intervals from (293.15 to 413.15) K in the pressure range from atmospheric pressure to 200 MPa using a 10 MPa step. The details of the method and technique used to determine speed of sound and density by an acoustic piezometer have been described previously.[12] This method makes possible measurements of the speed of sound and the density of a liquid at pressure up to 600 MPa in the temperature range from (223.15 to 523.15) K. The variation of acoustic path (L) with temperature and pressure was calculated from

$$L_{P,T} = L_0 \Omega_P \Omega_T$$

where L_0 = 24.807 mm is path length at temperature T_0 = 293.15 and pressure P_0 = 0.1 MPa:

$$\Omega_T = 1 + \alpha(T - 293)$$

$$\Omega_P = 1 - \frac{1 - 2\mu}{E} P$$

where μ, α, E, T, and P are Poisson's coefficient, coefficient of thermal expansion, and Young's modulus absolute temperature and pressure, respectively. The speed of sound was measured at frequencies of 1 and 5 MHz. Dispersion was not observed. The density was measured by an acoustic piezometer with an uncertainty of ± 0.3 %. The density at atmospheric pressure (P_0) was measured by Ostwald−Sprengel-type pycnometer, with a capacity of approximately 50 cm^3 with an uncertainty estimated to be ± 3 × 10^{-5} g·cm^{-3}. The temperature was measured by the platinum resistance thermometer with uncertainty of ± 0.01 K The acoustic piezometer was thermostated with a temperature stability of ± 0.01 K. The pressure was measured by dead-weight pressure gauge MP-2500 with relative uncertainty 0.02 %. The apparatus calibration was performed periodically.

Results and Discussion

The experimental results of the speed of sound (u) and density (ρ) in the liquid phase of 1-chlorohexane at various temperatures (T) and pressures (P) are listed in Table 1 and Table 2 and are plotted as a function of temperature and pressure in Figures 1

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Table 1. Speed of Sound (u) in the Liquid Phase for 1-Chlorohexane at Various Temperatures (T) and Pressures (P)

	u/m·s^{-1} at T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
0.1	1219.1	1140.7	1068.8	995.0	922.9	853.3	784.0
5.00	1240.5	1166.4	1097.1	1026.2	957.0	893.8	829.4
9.91	1264.5	1191.8	1124.4	1055.4	989.6	928.6	867.7
19.72	1310.0	1240.1	1176.0	1110.7	1050.4	993.2	938.1
29.53	1352.6	1285.3	1224.0	1162.0	1105.8	1051.8	1001.1
39.34	1392.6	1327.6	1268.8	1209.8	1156.5	1105.2	1057.7
49.15	1430.1	1367.4	1310.8	1254.5	1203.2	1154.2	1109.0
58.96	1465.7	1405.0	1350.4	1296.3	1246.3	1199.4	1155.8
68.77	1499.3	1440.6	1387.7	1335.8	1286.9	1241.4	1198.9
78.58	1531.5	1474.6	1423.2	1373.0	1324.8	1280.8	1239.1
88.39	1562.3	1507.0	1457.0	1408.3	1360.8	1318.0	1276.9
98.2	1591.9	1538.0	1489.4	1441.9	1395.1	1353.3	1312.8
108.0	1620.6	1567.9	1520.4	1474.0	1427.9	1387.2	1347.4
117.8	1648.2	1596.7	1550.3	1504.7	1459.6	1419.7	1380.6
127.6	1675.2	1624.5	1579.1	1534.3	1490.1	1451.2	1413.0
137.4	1701.5	1651.4	1607.0	1562.7	1519.6	1481.6	1444.5
147.2	1727.1	1677.5	1633.9	1590.1	1548.1	1511.1	1475.2
157.1	1752.2	1702.6	1659.9	1616.4	1575.5	1539.5	1504.9
166.9	1776.7	1726.9	1684.9	1641.8	1601.7	1566.9	1533.7
176.7	1800.6	1750.3	1708.9	1666.1	1626.5	1592.8	1560.9
186.5	1824.0	1772.6	1731.8	1689.4	1649.5	1617.2	1586.4
196.3	1846.5	1793.6	1753.5	1711.4	1670.6	1639.7	1609.7

Table 2. Density (ρ) in the Liquid Phase for 1-Chlorohexane at Various Temperatures (T) and Pressures (P)

	ρ/kg·m^{-3} at T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
0.1	878.5	859.4	840.3	821.3	802.2	780.7	759.1
5.00	884.2	865.0	847.1	828.1	809.3	789.2	769.6
9.91	887.0	869.8	851.9	833.7	815.2	796.7	777.6
19.72	894.7	878.3	861.5	844.5	827.4	810.5	793.3
29.53	901.8	886.2	870.3	854.3	838.3	822.6	806.8
39.34	908.4	893.4	878.3	863.1	848.0	833.3	818.6
49.15	914.6	900.1	885.7	871.2	856.9	843.0	829.2
58.96	920.4	906.4	892.6	878.7	865.0	851.8	838.7
68.77	925.9	912.3	899.0	885.6	872.5	859.8	847.4
78.58	931.1	917.9	905.0	892.1	879.4	867.2	855.3
88.39	936.0	923.1	910.7	898.2	885.9	874.1	862.7
98.2	940.7	928.1	916.0	903.8	891.9	880.6	869.5
108.0	945.1	932.8	921.1	909.2	897.6	886.6	875.8
117.8	949.4	937.3	925.9	914.3	903.0	892.3	881.8
127.6	953.4	941.6	930.4	919.1	908.1	897.6	887.4
137.4	957.3	945.7	934.8	923.7	912.9	902.7	892.7
147.2	961.1	949.7	939.0	928.1	917.5	907.5	897.8
157.1	964.7	953.5	943.0	932.3	921.9	912.1	902.5
166.9	968.1	957.1	946.8	936.3	926.1	916.4	907.1
176.7	971.5	960.6	950.5	940.1	930.1	920.6	911.4
186.5	974.7	964.0	954.0	943.8	934.0	924.6	915.6
196.3	977.9	967.2	957.4	947.4	937.7	928.4	919.5

and 2, respectively. The data presented in Table 1 and Table 2 have been fitted by the following polynomial for each isotherm:

$$Y = \sum_{i=0}^{4} A_i (P/\text{MPa})^i \tag{1}$$

where Y is u (m·s^{-1}) or ρ (kg·m^{-3}), P is pressure, and A_i are the adjustable parameters. All the measured data were used in the fitting process. The values of coefficients (A_i) were calculated by least-squares method. Standard deviation $\sigma(Y)$ of u and ρ, defined by

$$\sigma(Y) = [\{\sum_{i=1}^{n}(Y_{\text{obs}} - Y_{\text{cal}})^2\}/\{(n-p)\}]^{1/2} \tag{2}$$

where Y_{obs} and Y_{cal} are the observed and calculated quantities as defined earlier, n is total number of experimental points, and p is the number estimated parameters. The values of parameters A_i of eq 1 and standard deviation $\sigma(Y)$ are given in Tables 3 and 4 at temperatures from 293.15 to 413.15 K, respectively. As can be seen from Figures 1 and 2, the speed of sound and density for 1-chlorohexane monotonically decrease with increase temperature along isobars and increases with increase of pressure

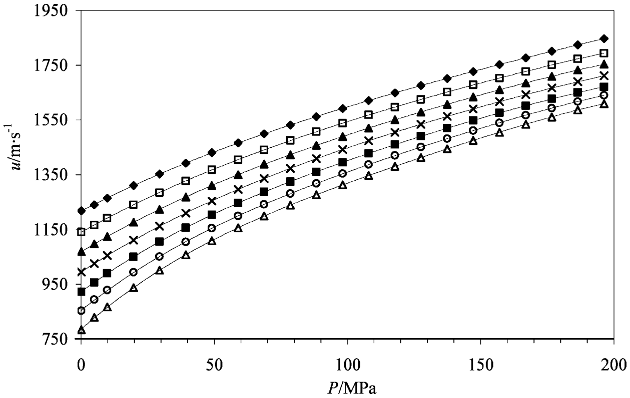

Figure 1. Speed of sound in the liquid phase of 1-chlorohexane as a function of pressure: ◆, 293.15 K; □, 313.15 K; ▲, 333.15 K; ×, 353.15 K; ■, 373.15 K; ○, 393.15 K; △, 413.15 K.

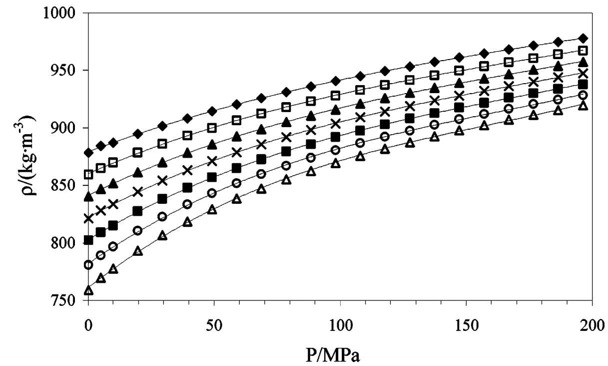

Figure 2. Density in the liquid phase of 1-chlorohexane as a function of pressure: ◆, 293.15 K; □, 313.15 K; ▲, 333.15 K; ×, 353.15 K; ■, 373.15 K; ○, 393.15 K; △, 413.15 K.

Table 3. Values of the Parameters of Equation 1 and Standard Deviation for Speed of Sound from (293.15 to 413.15) K

T/K	A_0	A_1	A_2	A_3	A_4	σ/m·s^{-1}
293.15	1216.93	5.05256	−0.01720	5.50529×10^{-5}	-7.78707×10^{-8}	1.61
313.15	1139.82	5.45839	−0.02005	7.06002×10^{-5}	-1.20424×10^{-7}	0.45
333.15	1068.24	5.88724	−0.02316	8.45021×10^{-5}	-1.46088×10^{-7}	0.21
353.15	994.782	6.34468	−0.02559	8.92393×10^{-5}	-1.46662×10^{-7}	0.51
373.15	922.109	7.16599	−0.03644	1.56479×10^{-4}	-2.94569×10^{-7}	0.29
393.15	854.429	7.79419	−0.04276	1.88515×10^{-4}	-3.52350×10^{-7}	1.92
413.15	785.450	8.69668	−0.05413	2.53466×10^{-4}	-4.81139×10^{-7}	2.30

Table 4. Values of the Parameters of Equation 1 and Standard Deviation for Density from (293.15 to 413.15) K

T/K	A_0	A_1	A_2	A_3	A_4	σ/kg·m^{-3}
293.15	879.032	0.85539	-3.0902×10^{-3}	9.101×10^{-6}	-1.270×10^{-8}	0.55
313.15	859.794	1.01956	-4.8448×10^{-3}	1.892×10^{-5}	-3.320×10^{-8}	0.61
333.15	840.895	1.14258	-5.6226×10^{-3}	2.172×10^{-5}	-3.744×10^{-8}	0.72
353.15	821.572	1.27548	-6.473×10^{-3}	2.451×10^{-5}	-4.085×10^{-8}	0.54
373.15	802.164	1.41122	-7.267×10^{-3}	2.663×10^{-5}	-4.243×10^{-8}	0.41
393.15	780.974	1.66314	-9.958×10^{-3}	4.110×10^{-5}	-7.171×10^{-8}	0.85
413.15	759.745	1.90517	-1.228×10^{-2}	5.247×10^{-5}	-9.295×10^{-8}	1.21

along isotherms. Changes of the sound speed and density values both with temperature and with pressure has nonlinear character along pronounced isotherms. And also, the maximal change of speed of sound and density values with change of pressure and temperatures occurs in the range of small pressures and high temperatures.

Isentropic compressibilities (k_S) of the 1-chlorohexane were calculated from the Laplace equation:

$$k_S = \frac{1}{\rho u^2} \tag{3}$$

where u is the sound velocity and ρ is the density. The values

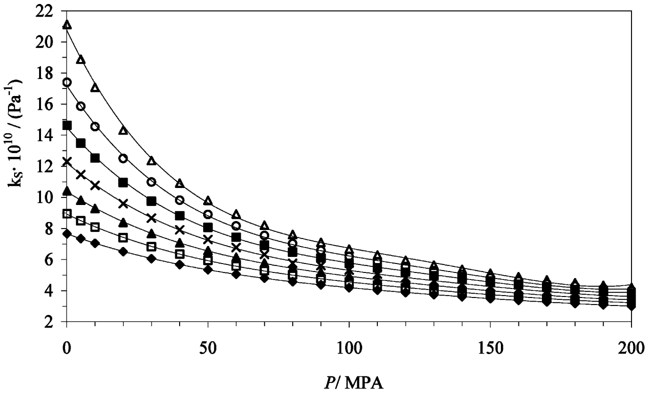

Figure 3. Pressure dependence (P) of isentropic compressibilities (k_S) in the liquid phase of 1-chlorohexane: ◆, 293.15 K; □, 313.15 K; ▲, 333.15 K; ×, 353.15 K; ■, 373.15 K; ○, 393.15 K; △, 413.15 K.

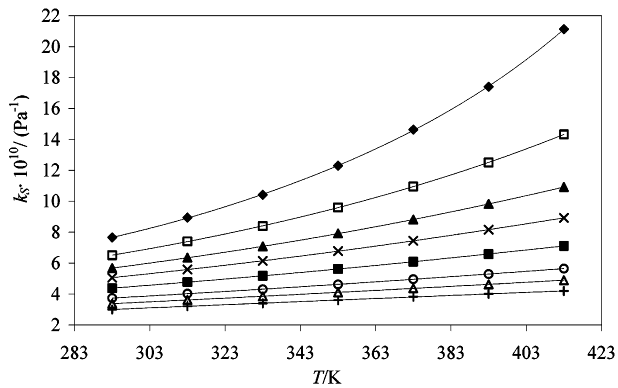

Figure 4. Temperature dependence (T) of isentropic compressibilities (k_S) in the liquid phase of 1-chlorohexane: ◆, 0.1 MPa; □, 20 MPa; ▲, 40 MPa; ×, 60 MPa; ■, 90 MPa; ○, 130 MPa; △, 160 MPa; +, 200 MPa.

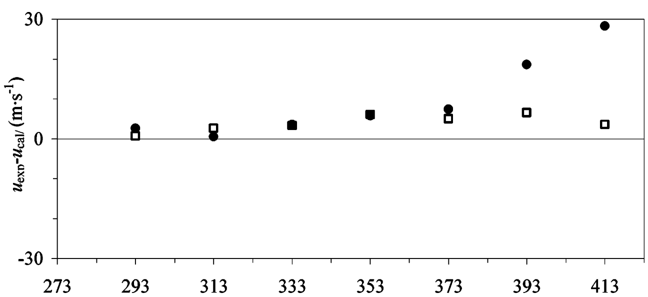

Figure 5. Deviations of calculated values of the speed of sound at P_0 from experimental values for 1-chlorohexane as function of temperature: □, eq 6; ■, eq 4.

of isentropic compressibilities (k_S) for 1-chlorohexane as a function of pressure at constant temperatures and as a function of temperature at constant pressures are plotted in Figures 3 and 4, respectively. The uncertainty of calculated of values for isentropic compressibilities $k_S \pm 1$ %. The isentropic compressibility carries more information on the strength of intermolecular interaction in liquid. It is well-known that the larger strength of intermolecular interaction corresponds to a lower isentropic compressibility. As was shown in ref 10, the isentropic compressibility of haloalkanes along the saturation line is less than the isentropic compressibility of n-alkanes corresponding to them. From Figure 5, it follows that, along isotherms with an increase in pressure, the strength of intermolecular interaction increases for 1-chlorohexane. From Figure 3, it follows that, along isobars with an increase in temperature, intensity of intermolecular interaction decreases for 1-chlorohexane.

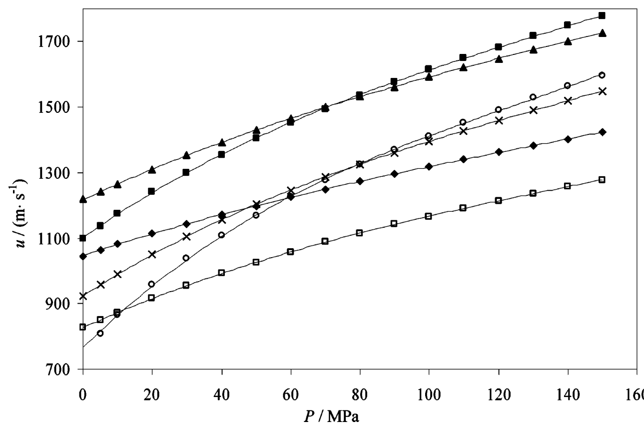

Figure 6. Speed of sound in the liquid phase of hexane, 1-iodohexane, and 1-chlorohexane as a function of pressure. 1-Iodohexane (ref 9): ◆, 293.15 K; □, 373.15 K. 1-Chlorohexane: ▲, 293.15 K; ×, 373.15 K. Hexane (ref 16): ■, 293.15 K; ○, 373.15 K.

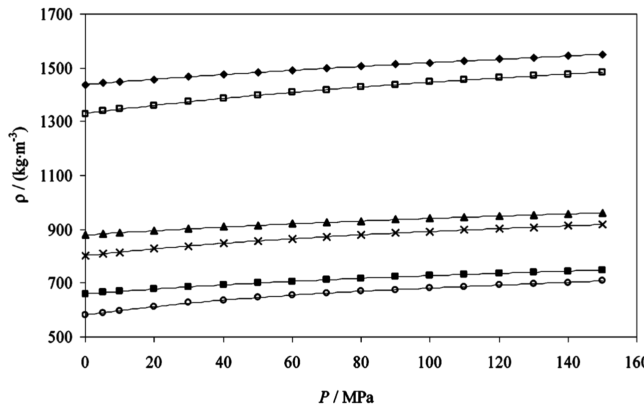

Figure 7. Density in the liquid phase of hexane, 1-iodohexane, and 1-chlorohexane as a function of pressure. 1-Iodohexane (ref 9): ◆, 293.15 K; □, 373.15 K. 1-Chlorohexane: ▲, 293.15 K; ×, 373.15 K. Hexane (ref 16): ■, 293.15 K; ○, 373.15 K.

Table 5. Values of the Parameters of Equation 4 and Standard Deviation (σ)

T/K	u_0/m·s^{-1}	K/m^4·kg^{-1}·s^{-1}	σ/m^3·s^{-3}
293.15	1216.5	22.41362	3.4·10^7
313.15	1140.2	21.55752	3.2·10^7
333.15	1065.2	20.99528	2.6·10^7
353.15	989.2	20.31394	1.7·10^7
373.15	915.5	19.58134	2.8·10^7
393.15	839.3	19.07018	2.2·10^7
413.15	761.3	18.52326	3.1·10^7

Table 6. Values of the Parameters of Equation 6 and Standard Deviation (σ)

T/K	u_0/m·s^{-1}	K_0/m^4·kg^{-1}·s^{-1}	α/m^5·kg^{-2}·s	σ/m^3·s^{-3}
293.15	1218.4	22.1497	1.310×10^{-9}	2.3·10^7
313.15	1138.1	21.8074	-1.240×10^{-9}	2.4·10^7
333.15	1065.5	20.9656	1.473×10^{-10}	1.9·10^7
353.15	988.9	20.3403	-1.313×10^{-10}	2.0·10^7
373.15	917.9	19.3949	9.251×10^{-10}	2.3·10^7
393.15	851.3	18.2744	3.950×10^{-9}	2.1·10^7
413.15	786.0	17.1530	6.802×10^{-9}	3.0·10^7

Pan'kevich et al.[13,14] discussed a linear relationship between u^3 and P:

$$(u/\text{m·s}^{-1})^3 = (u_0/\text{m·s}^{-1})^3 + K((P - P_0)/\text{Pa}) \qquad (4)$$

where u is the speed of sound at pressure (P), u_0 is the speed of sound at atmospheric pressure (P_0), and K is the pressure-independent constant. The values of coefficients u_0 and K for 1-chlorohexane were calculated by the least-squares method and presented in Table 5. In the same place the values of standard

Table 7. Isobaric Thermal Expansion Coefficient (α_P) in the Liquid Phase for 1-Chlorohexane at Various Temperatures (T) and Pressures (P)

	$\alpha_P \times 10^3$/K^{-1} at T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
0.1	1.086	1.111	1.136	1.183	1.265	1.350	1.436
5.00	1.021	1.064	1.085	1.140	1.203	1.265	1.307
9.91	0.975	1.010	1.061	1.102	1.134	1.178	1.219
19.72	0.927	0.946	0.982	1.011	1.027	1.050	1.079
29.53	0.881	0.889	0.917	0.938	0.945	0.956	0.977
39.34	0.841	0.842	0.863	0.879	0.878	0.881	0.896
49.15	0.805	0.802	0.816	0.828	0.822	0.820	0.831
58.96	0.772	0.766	0.776	0.787	0.777	0.770	0.778
68.77	0.744	0.736	0.742	0.750	0.739	0.729	0.735
78.58	0.719	0.710	0.712	0.719	0.708	0.694	0.698
88.39	0.693	0.683	0.683	0.692	0.681	0.663	0.668
98.2	0.677	0.663	0.663	0.669	0.650	0.635	0.635
108.0	0.654	0.641	0.640	0.649	0.629	0.613	0.615
117.8	0.637	0.624	0.620	0.629	0.609	0.593	0.593
127.6	0.621	0.608	0.604	0.609	0.592	0.576	0.575
137.4	0.605	0.592	0.587	0.595	0.575	0.558	0.557
147.2	0.593	0.579	0.574	0.582	0.561	0.542	0.541
157.1	0.580	0.566	0.561	0.568	0.547	0.530	0.529
166.9	0.567	0.553	0.548	0.555	0.538	0.518	0.518
176.7	0.557	0.543	0.538	0.545	0.524	0.507	0.506
186.5	0.547	0.534	0.528	0.532	0.514	0.498	0.495
196.3	0.536	0.526	0.515	0.522	0.507	0.490	0.488

Table 8. Isothermal Compressibility (k_T) in the Liquid Phase for 1-Chlorohexane at Various Temperatures (T) and Pressures (P)

	$k_T \times 10^{10}$/Pa^{-1} at T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
0.1	10.00	11.54	13.29	15.47	18.15	21.47	25.65
5.00	9.37	10.90	12.30	14.41	16.60	19.46	22.98
9.91	8.87	10.17	11.71	13.33	15.20	17.88	20.92
19.72	8.25	9.25	10.59	12.15	13.78	15.92	18.32
29.53	7.58	8.51	9.64	10.86	12.25	13.81	15.60
39.34	7.04	7.76	8.75	9.76	10.94	12.20	13.64
49.15	6.55	7.21	8.07	8.95	9.90	10.96	12.09
58.96	6.13	6.72	7.44	8.18	9.00	9.84	10.83
68.77	5.78	6.30	6.88	7.55	8.24	8.93	9.77
78.58	5.42	5.88	6.46	7.07	7.61	8.23	8.93
88.39	5.13	5.52	6.03	6.50	7.05	7.67	8.23
98.2	4.83	5.23	5.67	6.07	6.55	7.09	7.51
108.0	4.60	4.92	5.38	5.70	6.03	6.59	7.02
117.8	4.37	4.69	5.01	5.31	5.71	6.16	6.58
127.6	4.13	4.45	4.78	5.11	5.44	5.79	6.13
137.4	3.95	4.28	4.61	4.87	5.14	5.48	5.83
147.2	3.76	4.11	4.37	4.63	4.90	5.18	5.45
157.1	3.62	3.87	4.13	4.40	4.66	4.87	5.15
166.9	3.48	3.70	3.96	4.16	4.42	4.63	4.91
176.7	3.40	3.60	3.79	3.98	4.25	4.46	4.66
186.5	3.29	3.43	3.65	3.87	4.08	4.22	4.44
196.3	3.20	3.31	3.50	3.76	3.98	4.10	4.32

Table 9. Temperature Coefficient of Pressure at Constant Volume ($(\partial P/\partial T)_V$) in the Liquid Phase for 1-Chlorohexane at Various Temperatures (T) and Pressures (P)

	$(\partial P/\partial T)_V$/MPa·K^{-1} at T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
0.1	1.086	1.111	1.136	1.183	1.265	1.350	1.436
5.00	1.021	1.064	1.085	1.140	1.203	1.265	1.307
9.91	0.975	1.010	1.061	1.102	1.134	1.178	1.219
19.72	0.927	0.946	0.982	1.011	1.027	1.050	1.079
29.53	0.881	0.889	0.917	0.938	0.945	0.956	0.977
39.34	0.841	0.842	0.863	0.879	0.878	0.881	0.896
49.15	0.805	0.802	0.816	0.828	0.822	0.820	0.831
58.96	0.772	0.766	0.776	0.787	0.777	0.770	0.778
68.77	0.744	0.736	0.742	0.750	0.739	0.729	0.735
78.58	0.719	0.710	0.712	0.719	0.708	0.694	0.698
88.39	0.693	0.683	0.683	0.692	0.681	0.663	0.668
98.2	0.677	0.663	0.663	0.669	0.650	0.635	0.635
108.0	0.654	0.641	0.640	0.649	0.629	0.613	0.615
117.8	0.637	0.624	0.620	0.629	0.609	0.593	0.593
127.6	0.621	0.608	0.604	0.609	0.592	0.576	0.575
137.4	0.605	0.592	0.587	0.595	0.575	0.558	0.557
147.2	0.593	0.579	0.574	0.582	0.561	0.542	0.541
157.1	0.580	0.566	0.561	0.568	0.547	0.530	0.529
166.9	0.567	0.553	0.548	0.555	0.538	0.518	0.518
176.7	0.557	0.543	0.538	0.545	0.524	0.507	0.506
186.5	0.547	0.534	0.528	0.532	0.514	0.498	0.495
196.3	0.536	0.526	0.515	0.522	0.507	0.490	0.488

Table 10. Internal Pressure (P_i) in the Liquid Phase for 1-Chlorohexane at Various Temperatures (T) and Pressures (P)

	P_i/MPa at T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
0.1	318.3	301.4	284.7	270.0	260.0	247.1	231.2
5.00	314.6	300.6	288.9	274.5	265.4	250.6	230.0
9.91	312.2	301.0	291.9	281.9	268.3	248.9	230.8
19.72	309.7	300.4	289.1	274.1	258.3	239.6	223.6
29.53	311.1	297.6	287.6	275.3	258.3	242.7	229.3
39.34	311.0	300.6	289.5	278.8	260.3	244.3	232.2
49.15	310.9	299.0	287.9	277.8	260.7	245.2	234.7
58.96	310.2	297.7	288.3	281.0	263.1	248.9	238.1
68.77	308.8	296.8	290.6	281.9	266.1	252.2	241.8
78.58	310.8	299.7	288.6	280.7	268.6	252.9	244.4
88.39	307.7	299.3	288.5	287.8	272.1	251.8	246.9
98.2	312.6	299.3	291.1	290.9	272.4	253.6	251.0
108.0	308.4	299.3	288.0	294.0	281.3	257.8	254.1
117.8	309.2	298.3	294.4	300.5	280.0	260.6	254.5
127.6	312.9	300.1	293.4	293.3	278.1	263.7	259.9
137.4	311.9	295.4	287.1	294.2	279.7	262.7	257.5
147.2	315.5	293.5	290.6	296.3	279.8	264.0	263.2
157.1	313.2	300.4	295.3	299.4	280.9	270.9	267.9
166.9	310.5	301.2	294.0	304.4	286.9	272.9	269.4
176.7	304.1	295.9	296.4	306.7	283.5	270.3	271.3
186.5	301.1	301.0	295.8	299.1	284.1	277.2	274.3
196.3	294.9	301.6	294.0	293.8	278.9	273.6	270.3

deviation (σ) defined by the relation

$$\sigma = [\{\sum_{i=1}^{n}(u^3_{\text{obsd}} - u^3_{\text{calcd}})^2\}/\{(n-p)\}]^{1/2}$$

are presented. However, as was shown later[15] parameter K is slightly linearly increase with increasing pressure at temperatures greater than 333 K

$$K = K_0[1 + \alpha(P - P_0)] \quad (5)$$

where K_0 and α are new constants. A new relationship between u^3 and P can be obtained by combining eqs 4 and 5:

$$(u/\text{m·s}^{-1})^3 = (u_0/\text{m·s}^{-1})^3 + K_0((P - P_0)/\text{Pa}) + K_1((P - P_0)/\text{Pa})^2 \quad (6)$$

The values of parameters u_0, K_0, $K_1 = \alpha K_0$ and standard deviation (σ) for 1-chlorohexane determined by the least-squares method are listed in Table 6. Deviations of calculated by eqs 4 and 6, values of the speed of sound at P_0 from experimental values for 1-chlorohexane as function of temperature presented in Figure 5. As can be seen from Figure 5, calculations speed of sound with help eq 6 is preferred than with help eq 4.

By comparison the pressure dependences of speed of sound and density at 293.15 K and 373.15 K for 1-chlorohexane, 1-iodohexane, and hexane in Figures 6 and 7 are presented. For construction, Figures 6 and 7 were used data mentioned Daridon at al.[16] for hexane and our resent work[9] for 1-iodohexane. As can be seen from Figures 6 and 7, substitution of hydrogen atom in *n*-alkanes by atoms chlorine or iodine influence markedly on investigation properties.

In addition, several other thermophysical properties such as the isothermal compressibility (k_T), the isobaric thermal expansion coefficient (α_P), temperature coefficient of pressure at constant volume ($(\partial P/\partial T)_V$), and internal pressure (P_i) can be evaluated from the data reported here. The isobaric thermal expansion coefficient

$$\alpha_P = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P \quad (7)$$

and isothermal compressibility

$$k_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_T \qquad (8)$$

were calculated from numerical differentiation of the experimental density's data. The calculated values of α_P and k_T are presented in Tables 7 and 8. Calculations of values (see Tables 9 and 10) temperature coefficient of pressure at constant volume ($(\partial P/\partial T)_V$), and internal pressure (P_i) were carried out with the following equations:

$$\left(\frac{dP}{dT}\right)_V = \frac{\alpha_P}{k_T} \qquad (9)$$

$$P_i = \left(\frac{dE}{dV}\right)_T = T\frac{\alpha_P}{k_T} - P \qquad (10)$$

The uncertainties of calculated of values α_P, k_T, $(\partial P/\partial T)_V$, and P_i were less 5 % for isobaric thermal expansion coefficient, isothermal compressibilities and near 6 % for temperature coefficient of pressure at constant volume and internal pressure.

As can be seen for all isotherms in the range of temperatures and pressures the values of $(\partial P/\partial T)_V$ increase practically linearly with increasing pressure with constant of proportionality equal 0.003 K^{-1}. The values of internal pressure are practically constant along isotherms (293.15 to 333.15) K and lightly increase along isotherms (353.15 to 413.15) K increasing pressure.

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