Speed of Sound of 2-Methylpentane, 2,3-Dimethylpentane, and 2,2,4-Trimethylpentane from (293.15 to 373.15) K and up to 150 MPa

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In this work, ultrasonic velocity measurements in the compressed liquid phase of three branched alkanes (2-methylpentane, 2,3-dimethylpentane, and 2,2,4-trimethylpentane) from (293.15 to 373.15) K and for pressures ranging up to 150 MPa are presented. These results were used to estimate various thermophysical properties such as density and isentropic or isothermal compressibilities in the same range of pressure and temperature.

Introduction

The accurate measurement of ultrasonic velocity can play an important role in the characterization of the effect of pressure on thermodynamic properties of liquids if it coincides perfectly with the speed of sound within the low-frequency limit (c). In this case, achieved below 10 MHz for alkanes,[1,2] the speed of sound is a purely thermodynamic property linked to density (ρ) and isentropic compressibility (κ_S) through the Newton−Laplace's equation:

$$\kappa_S = \frac{1}{\rho c^2} \tag{1}$$

It is therefore related to the isothermal compressibility (κ_T):

$$\kappa_T = \kappa_S + \frac{T\alpha_p{}^2}{\rho C_p} \tag{2}$$

and to the change of density (ρ) with respect to pressure:

$$\rho(P, T) - \rho(P_{ref}, T) = \int_{P_{ref}}^{P} 1/c^2 \, dP + T\int_{P_{ref}}^{P} (\alpha_p{}^2/C_p) \, dP \tag{3}$$

where C_p is the heat capacity at constant pressure and α_p is the isobaric thermal expansion coefficient. Then, acoustic measurements that can be performed with a high degree of accuracy including at high pressures provide an easy and precise way for determining density and derived properties (κ_S and κ_T), which are frequently required in the design of chemical engineering processes and which are difficult to measure directly with a good precision. Thus, extensive works have been performed to measure the speed of sound in liquid alkanes and to determine volumetric and even calorimetric properties under high pressure from acoustic measurements. However, these systematic studies have mainly focused on linear alkanes. We have therefore measured, in the present work, the speed of sound in a series of pentane parent chains with a variable number of methyl branches in order to extend these investigations to branched alkanes. More precisely, ultrasonic measurements were carried out in the pressure range of (0.1 to 150) MPa and in the temperature range of (293.15 to 373.15) K in 2-methylpentane, 2,3-dimethylpentane, and 2,2,4-trimethylpentane. Accurate density (ρ) and isentropic (κ_S) and isothermal (κ_T) compressibilities were deduced from these ultrasonic measurements.

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Experimental Section

Ultrasonic wave velocities were measured to a maximum pressure of 150 MPa using a pulse transmission−reflection apparatus working at 3 MHz. The apparatus, which has been described previously in detail,[3] consists of an autoclave cell closed at both ends by two rods on which piezoelectric (PZT) elements are housed. One acts as a pulse transmitter/receiver whereas the second acts as a receiver only. The ultrasonic velocity was deduced from the measurement, by direct chronometry,[4] of the time-of-flight of the wave through the cell. This time was corrected for the time delay through both rods (measured by reflection) in order to estimate the traveling time in the liquid sample. The length of the sample path was determined precisely at each pressure and temperature condition by calibration with water.[5,6]

To keep constant the temperature, the cell was fully immerse in a liquid bath controlled by a thermostat with stability of ± 0.02 K. The temperature was measured by means of a calibrated platinum probe (Pt100) placed inside the high-pressure vessel and connected to a digital panel (AOIP brand). The uncertainty in the temperature measurements is estimated to be ± 0.1 K.

The pressure was generated by a high-pressure pneumatic pump and measured by a high-pressure transducer frequently checked against a dead-weight tester to an accuracy of better than 0.02 % full scale. All compounds were supplied by Sigma with a mole fraction purity higher than 99 % and used without further purification.

Results and Discussion

Speed of sound measurements were performed along isotherms spaced at 10 K intervals from 293.15 to 373.15 K in the pressure range from atmospheric pressure to 150 MPa using 10 MPa steps. The data were taken exclusively in the liquid state, which leaves aside values above the boiling temperature at atmospheric pressure. The speed

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Table 1. Speed of Sound (c) of the Three Branched Alkanes as a Function of Pressure and Temperature

	c/m·s^{-1} at T/K								
P/MPa	293.15	303.15	313.15	323.15	333.15	343.15	353.15	363.15	373.15
				2-Methylpentane					
0.1	1064.6	1016.5	971.8	927.3					
10	1145.5	1102.8	1061.7	1022.0	982.1	943.2	905.0	867.4	830.7
20	1215.4	1176.0	1138.5	1101.2	1065.4	1030.2	996.4	962.8	931.1
30	1277.6	1240.8	1205.5	1170.8	1137.2	1104.8	1073.6	1042.9	1013.0
40	1334.9	1299.5	1265.9	1233.9	1201.3	1170.9	1141.0	1112.8	1084.6
50	1386.9	1352.6	1321.2	1289.9	1260.2	1230.4	1201.8	1174.7	1148.2
60	1434.8	1403.0	1372.2	1342.1	1313.1	1284.6	1257.8	1231.7	1206.3
70	1480.4	1449.6	1419.4	1391.6	1363.4	1335.3	1309.7	1284.1	1259.6
80	1523.4	1492.9	1464.0	1436.0	1408.6	1381.8	1356.7	1332.7	1309.0
90	1564.0	1534.6	1506.3	1478.4	1452.5	1426.6	1402.3	1378.4	1354.6
100	1602.3	1573.5	1546.3	1519.2	1493.6	1468.3	1444.8	1421.9	1399.0
110	1638.5	1610.7	1584.2	1558.7	1532.6	1508.4	1485.1	1462.6	1440.8
120	1674.4	1646.9	1620.7	1595.2	1570.0	1546.2	1523.3	1501.1	1479.6
130	1708.1	1681.6	1655.7	1630.8	1605.9	1582.5	1560.0	1538.3	1517.1
140	1740.8	1714.3	1689.6	1664.2	1640.4	1617.2	1595.2	1573.9	1553.0
150	1771.8	1746.6	1721.4	1696.8	1673.0	1650.2	1628.8	1607.8	1587.5
				2,3-Dimethylpentane					
0.1	1149.5	1103.2	1061.2	1017.4	973.7	931.0	889.5	849.4	808.9
10	1220.2	1178.6	1138.0	1099.7	1061.7	1022.5	986.1	950.4	914.8
20	1284.8	1245.9	1207.8	1171.8	1136.5	1101.8	1067.4	1035.4	1003.1
30	1342.3	1306.5	1270.7	1236.2	1203.1	1170.5	1138.8	1108.4	1079.0
40	1396.2	1361.5	1327.2	1294.8	1263.1	1232.0	1201.8	1173.6	1145.4
50	1445.3	1411.9	1379.5	1348.2	1317.7	1287.5	1259.9	1232.3	1205.1
60	1491.9	1458.5	1428.2	1397.8	1368.8	1339.8	1312.3	1286.2	1260.3
70	1535.2	1503.4	1473.4	1444.3	1416.0	1388.3	1361.7	1336.7	1311.6
80	1576.5	1545.5	1516.6	1488.2	1460.6	1433.1	1407.9	1383.4	1358.8
90	1616.1	1585.9	1557.2	1529.5	1502.6	1476.4	1451.0	1427.8	1403.8
100	1653.0	1623.9	1595.8	1569.1	1542.8	1516.8	1492.5	1469.5	1446.4
110	1688.6	1660.0	1632.9	1606.4	1580.5	1555.6	1531.5	1508.7	1486.3
120	1723.2	1694.7	1668.4	1642.2	1617.1	1592.3	1569.2	1546.8	1524.6
130	1756.3	1728.8	1702.5	1676.9	1652.2	1627.9	1604.7	1583.0	1561.1
140	1788.0	1760.4	1735.5	1713.3	1685.7	1661.8	1639.3	1617.8	1596.4
150	1818.6	1792.3	1766.7	1742.2	1718.3	1694.8	1672.8	1650.9	1630.2
				2,2,4-Trimethylpentane					
0.1	1104.6	1061.7	1019.1	977.9	935.8	897.3	858.2	817.2	780.4
10	1178.5	1139.3	1100.9	1063.5	1026.6	992.6	958.0	924.3	891.0
20	1244.6	1208.6	1173.0	1138.8	1105.2	1071.6	1041.7	1011.1	980.7
30	1304.8	1270.2	1237.0	1204.7	1173.0	1142.7	1114.1	1085.5	1057.5
40	1358.5	1326.8	1295.2	1264.6	1234.2	1205.7	1178.7	1151.4	1125.2
50	1410.3	1378.5	1349.3	1319.0	1290.2	1262.9	1236.1	1211.3	1185.9
60	1458.1	1427.0	1397.6	1369.8	1341.8	1315.4	1290.4	1265.7	1242.1
70	1502.5	1472.6	1443.4	1416.6	1390.0	1363.5	1339.5	1316.6	1293.1
80	1544.7	1515.6	1487.6	1461.2	1434.9	1410.8	1386.8	1364.4	1341.5
90	1584.5	1556.4	1529.0	1503.4	1479.0	1453.6	1431.0	1408.2	1386.0
100	1622.6	1594.5	1568.7	1543.4	1519.0	1495.3	1472.5	1449.9	1428.5
110	1658.9	1632.1	1605.9	1581.4	1557.7	1534.0	1512.1	1490.6	1469.2
120	1694.0	1667.5	1641.7	1617.8	1594.1	1571.7	1549.6	1529.0	1508.2
130	1727.5	1701.6	1676.3	1653.1	1629.5	1607.2	1585.9	1565.5	1545.1
140	1760.1	1734.3	1709.4	1686.4	1663.5	1641.7	1620.5	1600.8	1580.3
150	1791.1	1766.4	1741.7	1718.6	1696.2	1675.0	1654.1	1634.2	1614.0

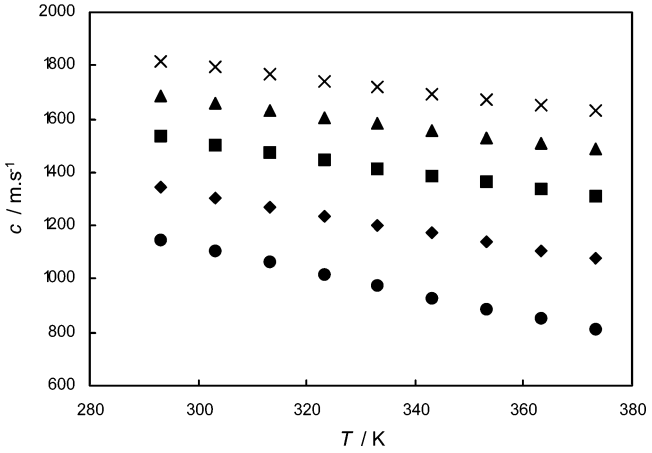

Figure 1. Speed of sound (c) of 2,3-dimethylpentane as a function of temperature (T) at the pressures ●, 0.1 MPa; ◆, 30 MPa; ■, 70 MPa; ▲, 110 MPa; ×, 150 MPa.

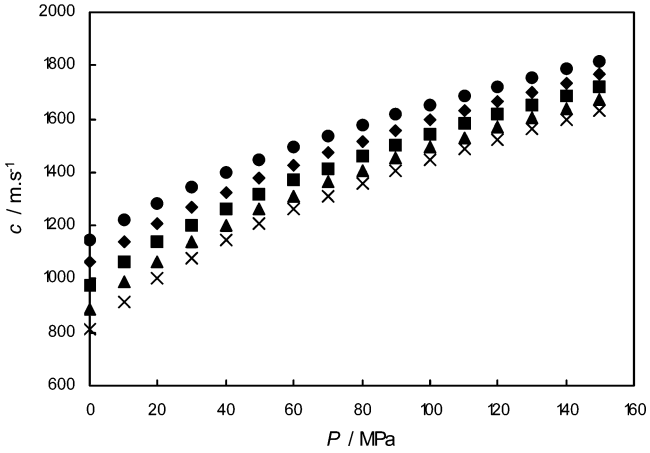

Figure 2. Speed of sound (c) of 2,3-dimethylpentane as a function of pressure (P) at the temperatures ●, 293.15 K; ◆, 313.15 K; ■, 333.15 K; ▲, 353.15 K; ×, 373.15 K.

of sound values obtained for these three branched alkanes are listed in Table 1. From a qualitative point of view, the behavior of the speed of sound versus pressure and temperature is similar, whatever the branched alkanes con-

Table 2. Comparison of Speed of Sound Values with Those Found in the Literature at Atmospheric Pressure

		c/m·s^{-1}	
compound	T/K	exptl	lit
2-methylpentane	298.15	1038.6	1041.4[7]; 1040.9[8]
2,3-dimethylpentane	293.15	1149.5	1150[9]
2,2,4-trimethylpentane	293.15	1104.6	1105[9]; 1102.2[10]
	298.15	1083.2	1080[11]
	303.15	1061.7	1061.6[10]; 1059[11]
	318.15	998.8	1002[11]

sidered. The case of 2,3-dimethylpentane can usefully illustrate the respective isobaric and isothermal variations of the speed of sound (Figures 1 and 2).

The speed of sound in these compounds was previously measured only at atmospheric pressure in a narrow temperature range, more precisely between 293.15 K and 318.15 K.[7−11] Comparisons of our data with those found in the literature are reported in Table 2. Our data displayed at T = 298.15 K and T = 318.15 K were interpolated by

Table 3. Parameters of Equations 4 to 6

parameters	2-methylpentane	2,3-dimethylpentane	2,2,4-trimethylpentane
A_0/m^{-2}·s2	5.36629×10^{-7}	$3.83441 \times 10-7$	1.24944×10^{-7}
A_1/m^{-2}·s^2·K^{-1}	-4.11860×10^{-9}	$-2.58250 \times 10-9$	-2.48060×10^{-10}
A_2/m^{-2}·s^2·K^{-2}	1.73312×10^{-11}	1.18850×10^{-11}	5.50814×10^{-12}
A_3/m^{-2}·s^2·K^{-3}	-1.93310×10^{-14}	-1.34100×10^{-14}	-7.45840×10^{-15}
B/m^{-2}·s^2·MPa^{-1}	2.96185×10^{-9}	2.44685×10^{-9}	2.96733×10^{-9}
C/m^{-2}·s^2·MPa^{-2}	-1.31730×10^{-11}	-1.03570×10^{-11}	-1.37380×10^{-11}
D/m^{-2}·s^2·MPa^{-3}	3.28206×10^{-14}	2.53720×10^{-14}	3.52930×10^{-14}
E_1/K^{-1}	-2.13380×10^{-3}	-2.01914×10^{-3}	-2.00992×10^{-3}
F/MPa^{-1}	9.83740×10^{-3}	8.93169×10^{-3}	9.90506×10^{-3}
AD %	-2.7×10^{-4}	1.8×10^{-4}	-5.9×10^{-3}
AAD %	5.4×10^{-2}	4.9×10^{-2}	5.9×10^{-2}
MD %	1.9×10^{-1}	2.1×10^{-1}	1.9×10^{-1}

Table 4. Density (ρ) of the Three Branched Alkanes as a Function of Pressure and Temperature

	ρ/kg·m^{-3} at T/K								
P/MPa	293.15	303.15	313.15	323.15	333.15	343.15	353.15	363.15	373.15
				2-Methylpentane					
0.1	653.2	643.7	634.2	624.5					
10	663.7	655.1	646.5	637.8	629.0	620.2	611.2	602.1	592.8
20	672.9	664.9	656.9	649.0	641.0	633.0	625.0	616.9	608.7
30	681.2	673.6	666.1	658.6	651.2	643.9	636.5	629.1	621.7
40	688.6	681.4	674.2	667.2	660.2	653.3	646.4	639.6	632.7
50	695.5	688.5	681.7	675.0	668.3	661.8	655.3	648.8	642.4
60	701.8	695.1	688.5	682.0	675.7	669.4	663.2	657.1	651.0
70	707.7	701.2	694.8	688.6	682.5	676.5	670.5	664.7	658.8
80	713.3	706.9	700.7	694.7	688.8	683.0	677.3	671.6	666.0
90	718.6	712.3	706.3	700.4	694.7	689.0	683.5	678.1	672.6
100	723.6	717.4	711.5	705.8	700.2	694.7	689.4	684.1	678.8
110	728.4	722.3	716.5	710.9	705.4	700.1	694.9	689.7	684.7
120	733.0	727.0	721.2	715.7	710.4	705.2	700.1	695.1	690.1
130	737.4	731.4	725.8	720.3	715.1	710.0	705.0	700.2	695.3
140	741.6	735.7	730.1	724.8	719.6	714.6	709.8	705.0	700.3
150	745.7	739.9	734.3	729.0	724.0	719.0	714.3	709.6	705.0
				2,3-Dimethylpentane					
0.1	694.3	686.4	677.5	667.8	657.7	647.5	637.7	628.6	620.6
10	702.6	695.8	688.0	679.4	670.3	661.0	651.9	643.3	635.7
20	709.9	704.0	697.1	689.4	681.0	672.4	663.8	655.6	648.2
30	716.4	711.2	705.1	698.1	690.5	682.4	674.2	666.2	658.9
40	722.3	717.7	712.2	705.9	698.9	691.3	683.5	675.7	668.4
50	727.8	723.7	718.7	712.9	706.4	699.4	691.9	684.3	677.1
60	732.8	729.1	724.6	719.3	713.3	706.7	699.6	692.2	685.0
70	737.5	734.2	730.0	725.2	719.7	713.5	706.7	699.5	692.4
80	741.9	738.9	735.1	730.6	725.5	719.7	713.3	706.3	699.3
90	746.1	743.3	739.8	735.7	731.0	725.6	719.4	712.7	705.9
100	750.1	747.5	744.3	740.5	736.1	731.0	725.2	718.7	712.0
110	753.9	751.4	748.5	744.9	740.9	736.1	730.6	724.4	717.9
120	757.5	755.2	752.4	749.2	745.4	741.0	735.8	729.8	723.5
130	761.0	758.8	756.2	753.2	749.7	745.5	740.6	734.9	728.8
140	764.3	762.3	759.8	757.0	753.8	749.9	745.2	739.8	733.8
150	767.5	765.6	763.3	760.7	757.6	754.0	749.6	744.4	738.7
				2,2,4-Trimethylpentane					
0.1	691.9	683.7	675.4	667.0	658.5	649.8	640.8	631.5	621.9
10	701.2	693.6	686.0	678.5	670.8	663.1	655.2	647.2	639.0
20	709.4	702.3	695.3	688.3	681.3	674.2	667.1	659.9	652.6
30	716.8	710.1	703.5	696.9	690.4	683.8	677.3	670.6	663.9
40	723.6	717.2	710.9	704.6	698.5	692.3	686.2	680.0	673.8
50	729.9	723.7	717.6	711.7	705.8	700.0	694.1	688.3	682.5
60	735.7	729.7	723.9	718.1	712.5	706.9	701.4	695.9	690.3
70	741.2	735.3	729.7	724.1	718.7	713.4	708.1	702.8	697.5
80	746.3	740.6	735.1	729.8	724.5	719.4	714.2	709.2	704.1
90	751.2	745.6	740.2	735.0	729.9	724.9	720.0	715.1	710.2
100	755.8	750.4	745.1	740.0	735.1	730.2	725.4	720.7	716.0
110	760.3	754.9	749.7	744.7	739.9	735.2	730.5	725.9	721.4
120	764.5	759.2	754.1	749.2	744.5	739.9	735.4	730.9	726.5
130	768.6	763.3	758.3	753.5	748.9	744.4	740.0	735.6	731.3
140	772.5	767.3	762.4	757.7	753.1	748.7	744.4	740.1	735.9
150	776.3	771.1	766.3	761.6	757.2	752.8	748.6	744.4	740.3

Table 5. Parameters of Equations 8 to 10

parameters	2-methylpentane	2,3-dimethylpentane	2,2,4-trimethylpentane
ρ_0/kg·m^{-3}	1.08960×10^{3}	-1.24237×10^{3}	1.14415×10^{3}
ρ_1/kg·m^{-3}·K^{-1}	−2.73451	1.90964×10^{1}	−2.98809
ρ_2/kg·m^{-3}·K^{-2}	6.58057×10^{-3}	-6.02298×10^{-2}	7.39773×10^{-3}
ρ_3/kg·m^{-3}·K^{-3}	-7.94980×10^{-6}	6.01179×10^{-5}	-8.41750×10^{-6}
a_0/m^3·kg^{-1}	-2.42130×10^{-4}	-5.61590×10^{-4}	-1.89550×10^{-4}
a_1/m^3·kg^{-1}·K^{-1}	7.30663×10^{-7}	3.32953×10^{-6}	4.76728×10^{-7}
a_2/m^3·kg^{-1}·K^{-2}	-1.34970×10^{-9}	-6.07830×10^{-9}	-9.00110×10^{-10}
b_0/MPa	3.35002×10^{2}	8.48995×10^{2}	3.28672×10^{2}
b_1/MPa·K^{-1}	−1.37617	−4.63047	−1.28833
b_2/MPa·K^{-2}	1.43414×10^{-3}	6.59823×10^{-3}	1.28625×10^{-3}
AD %	4.8×10^{-4}	-1.3×10^{-3}	-1.9×10^{-3}
AAD %	1.0×10^{-2}	1.8×10^{-2}	1.2×10^{-2}
MD %	5.8×10^{-2}	1.2×10^{-1}	3.3×10^{-2}

Table 6. Isothermal Compressibility (κ_T) of the Three Branched Alkanes as a Function of Pressure and Temperature

	κ_T/GPa^{-1} at T/K								
P/MPa	293.15	303.15	313.15	323.15	333.15	343.15	353.15	363.15	373.15
					2-Methylpentane				
0.1	1.767	1.953	2.159	2.400					
10	1.486	1.608	1.752	1.908	2.084	2.285	2.509	2.768	3.056
20	1.291	1.381	1.481	1.596	1.713	1.853	1.997	2.161	2.329
30	1.146	1.218	1.293	1.380	1.466	1.568	1.671	1.787	1.906
40	1.033	1.090	1.152	1.217	1.288	1.365	1.443	1.528	1.619
50	0.944	0.992	1.041	1.094	1.150	1.211	1.276	1.344	1.415
60	0.873	0.911	0.951	0.995	1.042	1.093	1.145	1.201	1.259
70	0.812	0.844	0.878	0.914	0.954	0.997	1.040	1.087	1.136
80	0.760	0.787	0.816	0.848	0.882	0.918	0.956	0.995	1.036
90	0.715	0.739	0.764	0.791	0.820	0.851	0.884	0.918	0.955
100	0.676	0.697	0.718	0.742	0.767	0.795	0.823	0.852	0.885
110	0.643	0.660	0.679	0.699	0.722	0.745	0.771	0.797	0.825
120	0.612	0.627	0.643	0.661	0.682	0.703	0.725	0.749	0.774
130	0.585	0.598	0.612	0.628	0.646	0.665	0.685	0.706	0.729
140	0.561	0.572	0.584	0.599	0.614	0.632	0.650	0.669	0.689
150	0.539	0.548	0.559	0.572	0.587	0.602	0.618	0.635	0.654
					2,3-Dimethylpentane				
0.1	1.298	1.502	1.710	1.918	2.127	2.318	2.489	2.644	2.800
10	1.110	1.262	1.424	1.583	1.735	1.876	1.986	2.073	2.149
20	0.970	1.091	1.223	1.351	1.474	1.585	1.675	1.730	1.769
30	0.866	0.962	1.068	1.177	1.282	1.379	1.453	1.499	1.524
40	0.784	0.862	0.951	1.045	1.138	1.222	1.289	1.331	1.348
50	0.718	0.783	0.857	0.938	1.021	1.096	1.157	1.202	1.219
60	0.664	0.718	0.781	0.852	0.925	0.995	1.054	1.097	1.116
70	0.618	0.664	0.718	0.780	0.846	0.910	0.967	1.006	1.030
80	0.579	0.618	0.664	0.719	0.778	0.839	0.892	0.934	0.959
90	0.545	0.578	0.619	0.667	0.721	0.776	0.828	0.869	0.899
100	0.516	0.545	0.580	0.623	0.671	0.722	0.771	0.813	0.844
110	0.490	0.515	0.546	0.584	0.628	0.675	0.721	0.763	0.796
120	0.466	0.489	0.516	0.550	0.590	0.634	0.677	0.718	0.752
130	0.445	0.465	0.490	0.520	0.556	0.596	0.638	0.677	0.713
140	0.426	0.444	0.466	0.492	0.526	0.563	0.602	0.640	0.676
150	0.409	0.425	0.445	0.470	0.499	0.533	0.570	0.607	0.643
					2,2,4-Trimethylpentane				
0.1	1.458	1.583	1.733	1.904	2.100	2.315	2.568	2.883	3.221
10	1.250	1.345	1.447	1.562	1.689	1.832	1.987	2.162	2.361
20	1.103	1.170	1.249	1.334	1.424	1.528	1.632	1.754	1.886
30	0.988	1.043	1.103	1.168	1.239	1.315	1.396	1.485	1.578
40	0.900	0.943	0.991	1.043	1.100	1.160	1.223	1.293	1.366
50	0.825	0.863	0.901	0.945	0.992	1.041	1.093	1.148	1.207
60	0.765	0.796	0.830	0.865	0.904	0.946	0.989	1.035	1.083
70	0.714	0.740	0.770	0.800	0.833	0.869	0.905	0.943	0.985
80	0.670	0.693	0.718	0.744	0.773	0.802	0.835	0.867	0.903
90	0.632	0.652	0.673	0.696	0.721	0.748	0.775	0.805	0.836
100	0.599	0.616	0.635	0.655	0.677	0.700	0.725	0.751	0.778
110	0.569	0.584	0.601	0.619	0.638	0.659	0.681	0.704	0.729
120	0.543	0.556	0.571	0.587	0.604	0.623	0.643	0.663	0.685
130	0.519	0.531	0.544	0.558	0.574	0.591	0.608	0.627	0.647
140	0.498	0.508	0.520	0.533	0.547	0.562	0.578	0.595	0.613
150	0.479	0.488	0.498	0.510	0.523	0.536	0.551	0.566	0.583

means of a polynomial function of temperature. The different values are consistent to less than 0.3 %.

The speed of sound values were smoothed as a function of temperature and pressure using a rational function which correlates $1/c^2$ with nine adjustable parameters:

$$c^2 = \frac{E + FP}{A + BP + CP^2 + DP^3} \tag{4}$$

where

$$A = A_0 + A_1T + A_2T^2 + A_3T^3 \quad (5)$$

and

$$E = 1 + E_1T \quad (6)$$

The sets of parameters determined by a least-squares method are listed in Table 3 along with the average deviation (AD %), the absolute average deviation (AAD %), and the maximum deviation (MD %). These deviations, which are less than the experimental error, show that the function leads to a good interpolation of the speed of sound data. This latter is therefore suitable to calculate analytically the integral of $1/c^2$ with respect to pressure in eq 3. By evaluating the last integral of eq 3 thanks to a predictor−corrector procedure,[3] it was then possible to evaluate the density as a function of pressure from speed of sound measurements. The uncertainty of the density determined by this method has been estimated to be less than ± 0.5 kg·m^{-3} on the basis of tests performed with hexane.[12] The atmospheric density data required to initiate the iterative procedure come from API Project 44,[13] whereas the atmospheric values of C_p result from the compilation of Zabranski et al.[14] For the highest volatile compound (i.e., 2-methylpentane), the saturation pressure was considered as the reference pressure instead of the atmospheric one. The density data derived from these speed of sound measurements are listed in Table 4. The full sets of data were correlated by means of a Tait-like equation:

$$\frac{1}{\rho} = \frac{1}{\rho_{\text{ref}}} + a \ln\left(\frac{P+b}{P_{\text{ref}}+b}\right) \quad (7)$$

in which a, b, and ρ_{ref} were correlated with temperature by means of polynomial functions:

$$\rho_{\text{ref}} = \rho_0 + \rho_1T + \rho_2T^2 + \rho_3T^3 \quad (8)$$

$$a = a_0 + a_1T + a_2T^2 \quad (9)$$

$$b = b_0 + b_1T + b_2T^2 \quad (10)$$

For 2,3-dimethylpentane and 2,2,4-trimethylpentane, parameters of eqs 8 to 10 were first evaluated alone by fitting atmospheric density data. The other parameters were then evaluated by an unweighted least squares procedure. For 2-methylpentane, all the parameters involved in eqs 8 to 10 were adjusted simultaneously by fitting the full set of density data, since its boiling point at atmospheric pressure is 334 K. The parameters ρ_i, a_i, and b_i for each compound are listed in Table 5 together with the related deviations.

For 2,2,4-trimethylpentane, our density values were confronted with those available under pressure in the literature and the comparison shows a very good agreement between the different sets of data. Our values were compared with those obtained by Hahn et al.[15] and Pádua et al.,[16] the absolute average deviation being of 0.03 % and 0.06 %, respectively.

The knowledge of c and ρ in the same temperature and pressure interval allowed the calculation of the isentropic and isothermal compressibilities from eqs 1 and 2 with an accuracy of 0.3 % and 1 %, respectively. The isothermal compressibilities values are summarized in Table 6.

The isothermal compressibility can also be derived from the fitted Tait equation:

$$\kappa_T = -\rho\frac{a}{P+b} \quad (11)$$

The comparison reveals excellent agreement between the two sets of compressibility data, those resulting from eq 2 on one hand and those resulting from the derivative of the Tait equation (eq 11) on the other hand. The two sets of data presents an average deviation (AD %) of 0.3 % and an absolute average deviation (AAD %) of 0.8 % for the three compounds.

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