

SUPPLEMENTARY MATERIAL TO
 **(p, ρ, T) properties of 1-octyl-3-methylimidazolium
tetrafluoroborate**

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THE CALCULATIONS

Isothermal compressibility $\kappa_T(p, T)$:

$$\kappa_T(p, T) = \frac{1}{\rho} \left(\frac{\partial p(T, \rho)}{\partial \rho} \right)_T^{-1} \quad (\text{S-1})$$

$$\kappa_T(p, T) = \frac{1}{2A(T)\rho^2 + 8B(T)\rho^8 + 12C(T)\rho^{12}} \quad (\text{S-2})$$

Isobaric thermal expansibility $\alpha_p(p, T)$:

$$\alpha_p(p, T) = \frac{1}{\rho} \left(\frac{\partial p(T, \rho)}{\partial T} \right)_\rho \left(\frac{\partial p(T, \rho)}{\partial \rho} \right)_T^{-1} \quad (\text{S-3})$$

$$\alpha_p(p, T) = \frac{A'(T) + B'(T)\rho^6 + C'(T)\rho^{10}}{2A(T) + 8B(T)\rho^6 + 12C(T)\rho^{10}} \quad (\text{S-4})$$

where: A' , B' , and C' are the derivatives of A , B and C , given by:

$$A'(T) = \sum_{i=1}^4 ia_i T^{i-1}, \quad (\text{S-5})$$

$$B'(T) = \sum_{i=1}^3 ib_i T^{i-1}, \quad (\text{S-6})$$

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$$C'(T) = \sum_{i=1}^3 ic_i T^{i-1}. \quad (\text{S-7})$$

Thermal pressure coefficient $\gamma(p, T)$:

$$\gamma(p, T) = \frac{\alpha_p(p, T)}{\kappa_T(p, T)} \quad (\text{S-8})$$

Internal pressure $p_{\text{int}}(p, T)$:

$$p_{\text{int}}(p, T) = \frac{T \cdot \alpha_p(p, T)}{\kappa_T(p, T)} - p \quad (\text{S-9})$$

Specific heat capacities [at constant pressure $c_p(p, T)$ and constant volume $c_v(p, T)$] at high pressures and temperatures:

$$c_v(p, T) = c_v(p_0, T) - T \int_{\rho_0}^{\rho} \left(\frac{\partial^2 p(T, \rho)}{\partial T^2} \right)_{\rho} \frac{d\rho}{\rho^2}, \quad (\text{S-10})$$

$$c_p(p, T) = c_v(p, T) + \frac{T \left(\frac{\partial p(T, \rho)}{\partial T} \right)_{\rho}^2}{\rho^2 \left(\frac{\partial p(T, \rho)}{\partial \rho} \right)_{T}}, \quad (\text{S-11})$$

$$c_p(p, T) - c_v(p, T) = \frac{\alpha_p^2(p, T) \cdot T}{\rho \cdot \kappa_T(p, T)} \quad (\text{S-12})$$

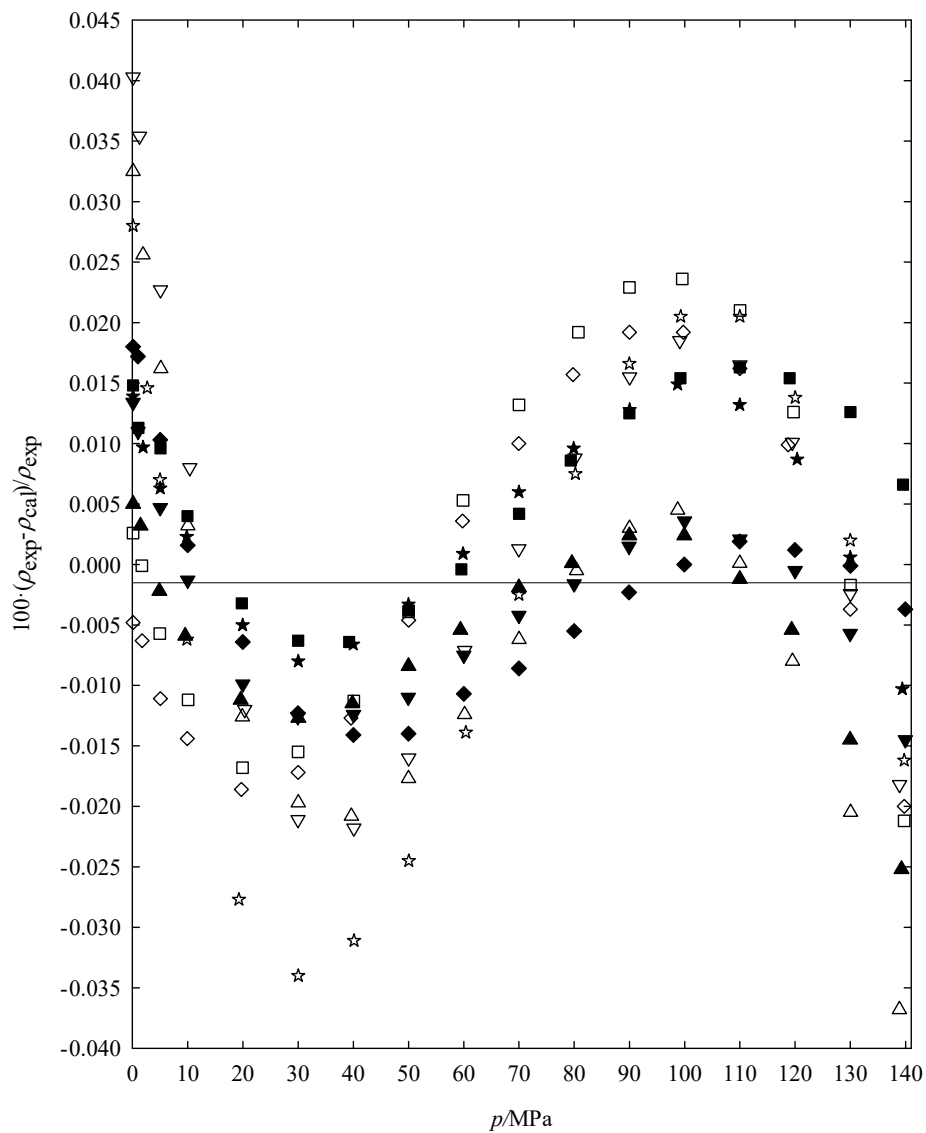


Fig. S-1. Plot of the deviations of the experimental density ρ_{exp} values of [OMIM][BF₄] from the density ρ_{cal} values calculated using Eqs. (2–5) versus pressure p at $T = (278.15 \text{ to } 413.14) \text{ K}$: \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.15 K; \triangle , 373.15 K; ∇ , 393.14 K and \star , 413.14 K.

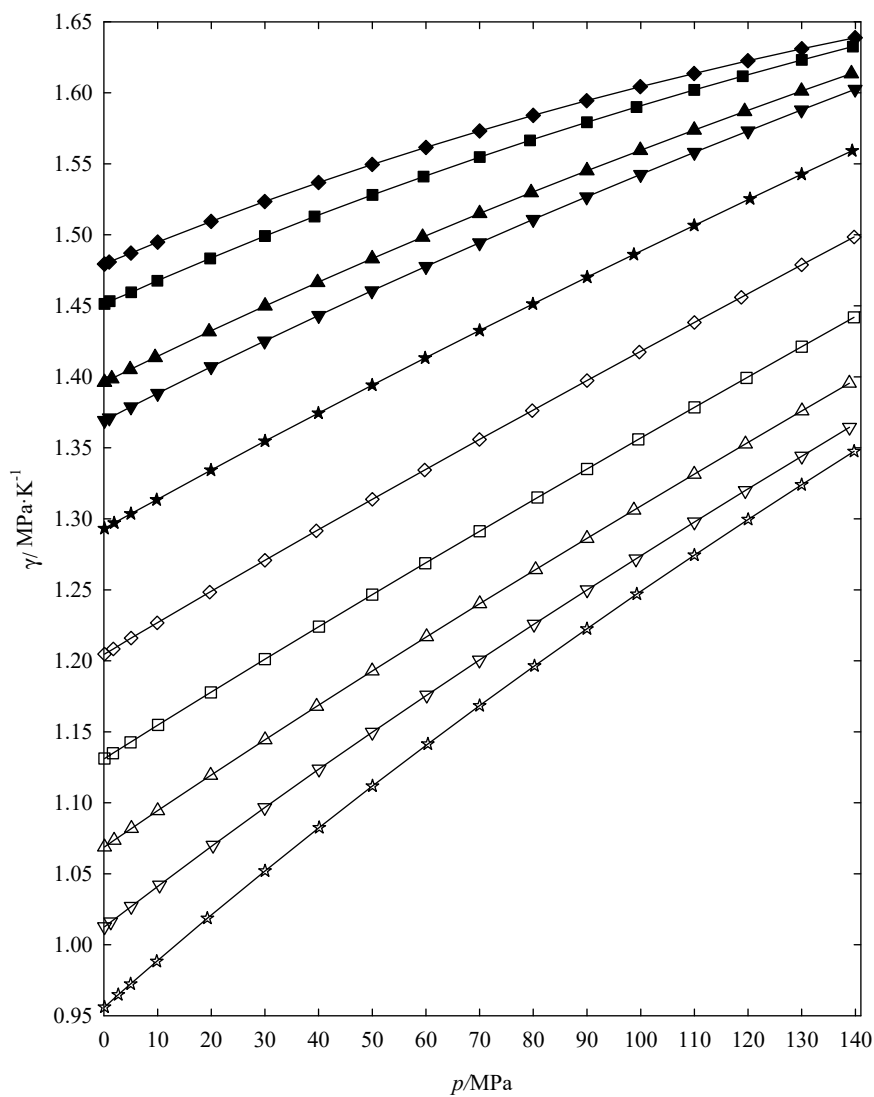


Fig. S-2. Plot of thermal coefficient of pressure $\gamma / \text{MPa}\cdot\text{K}^{-1}$ of $[\text{OMIM}][\text{BF}_4]$ versus pressure p : \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.16 K; \triangle , 373.16 K; \triangledown , 393.14 K; \star , 413.14 K; the lines are the best fit lines.

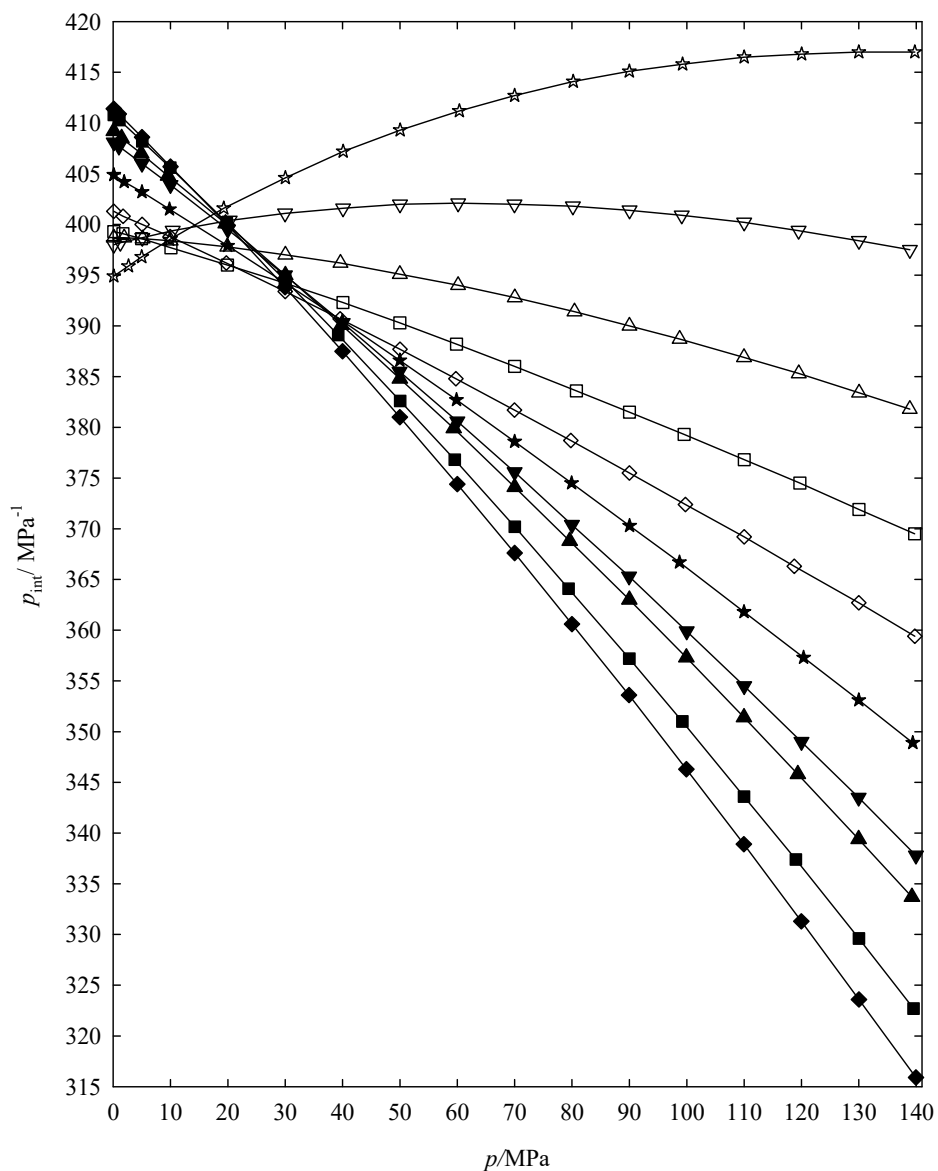


Fig. S-3. Plot of internal pressure p_{int} /MPa of [OMIM][BF₄] versus pressure p : ◆, 278.15 K; ■, 283.15 K; ▲, 293.15 K; ▼, 298.15 K; ★, 313.16 K; ◇, 333.15 K; □, 353.16 K; △, 373.16 K; ▽, 393.14 K; ☆, 413.14 K; the lines are the best fit lines.

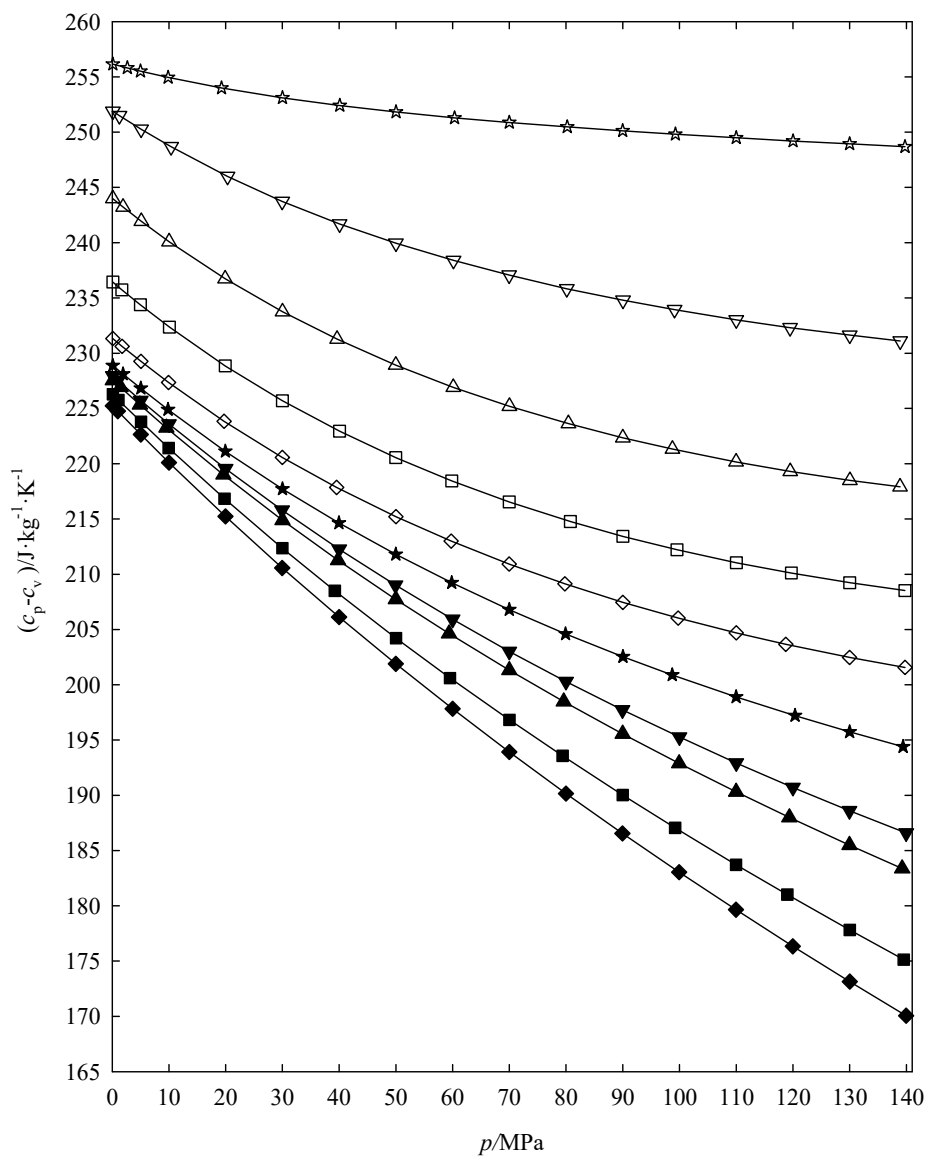


Fig. S-4. Plot of the difference in isobaric and isochoric heat capacities $(c_p - c_v) / \text{J kg}^{-1} \cdot \text{K}^{-1}$ of [OMIM][BF₄] versus pressure p : \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.16 K; \triangle , 373.16 K; ∇ , 393.14 K; \star , 413.14 K; the lines are the best fit lines.

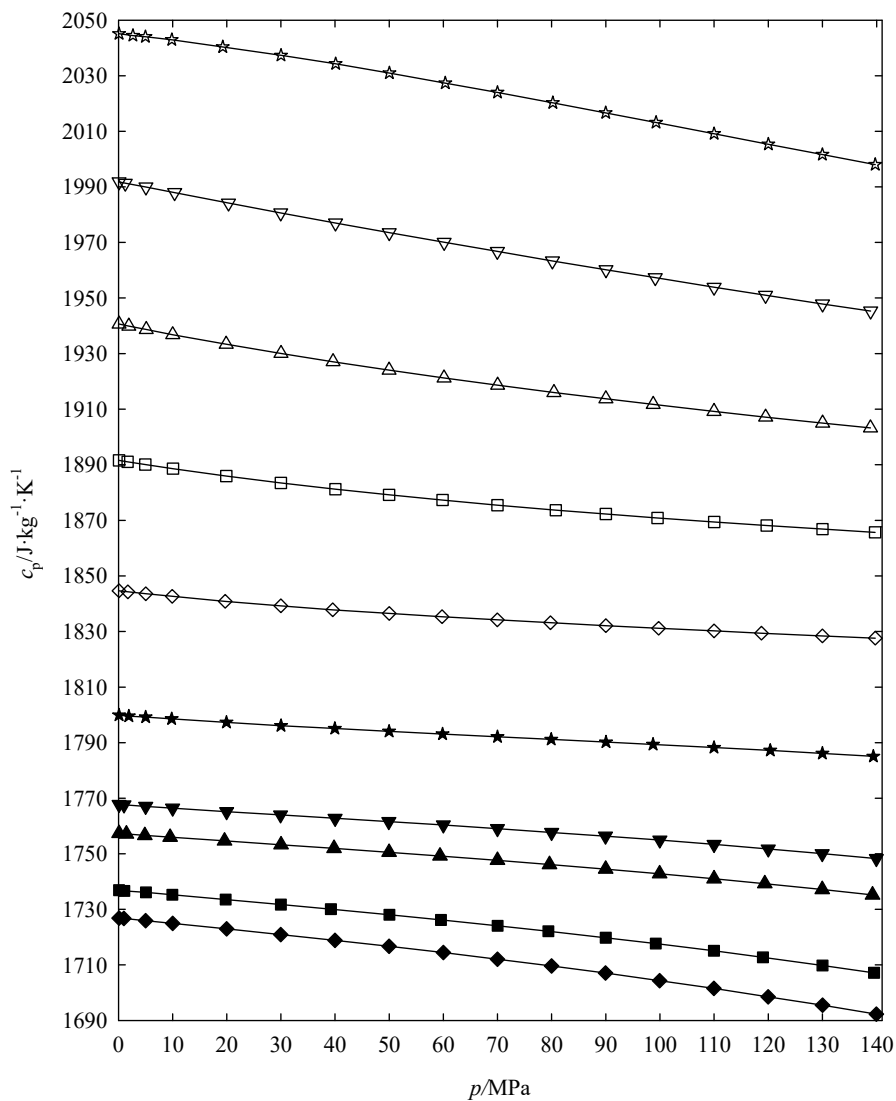


Fig. S-5. Plot of isobaric heat capacity $c_p / \text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$ of $[\text{OMIM}][\text{BF}_4]$ versus pressure p : \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.16 K; \triangle , 373.16 K; ∇ , 393.14 K; \star , 413.14 K; the lines are the best fit lines.

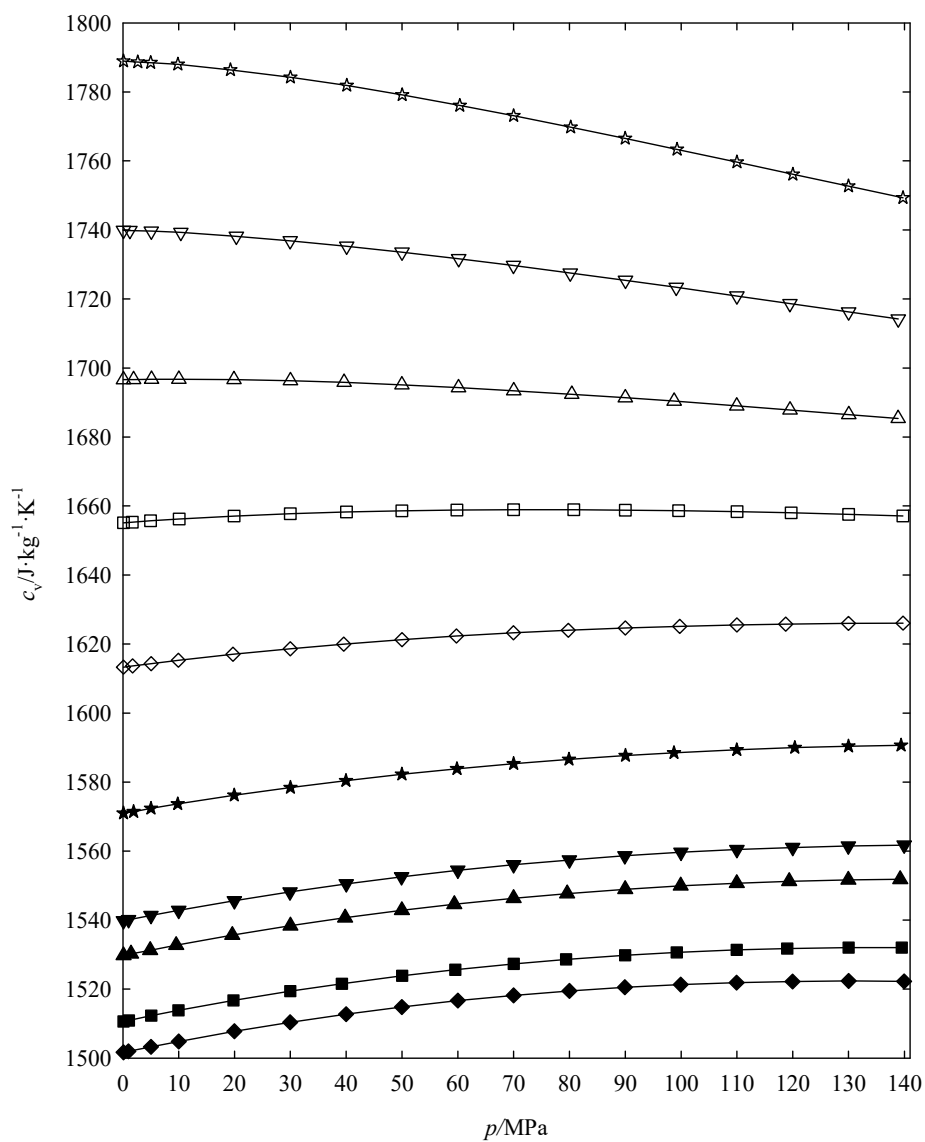


Fig. S-6. Plot of isochoric heat capacity c_v , / $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$ of $[\text{OMIM}][\text{BF}_4]$ versus pressure p : \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.16 K; \triangle , 373.16 K; \triangledown , 393.14 K; \star , 413.14 K; the lines are the best fit lines.

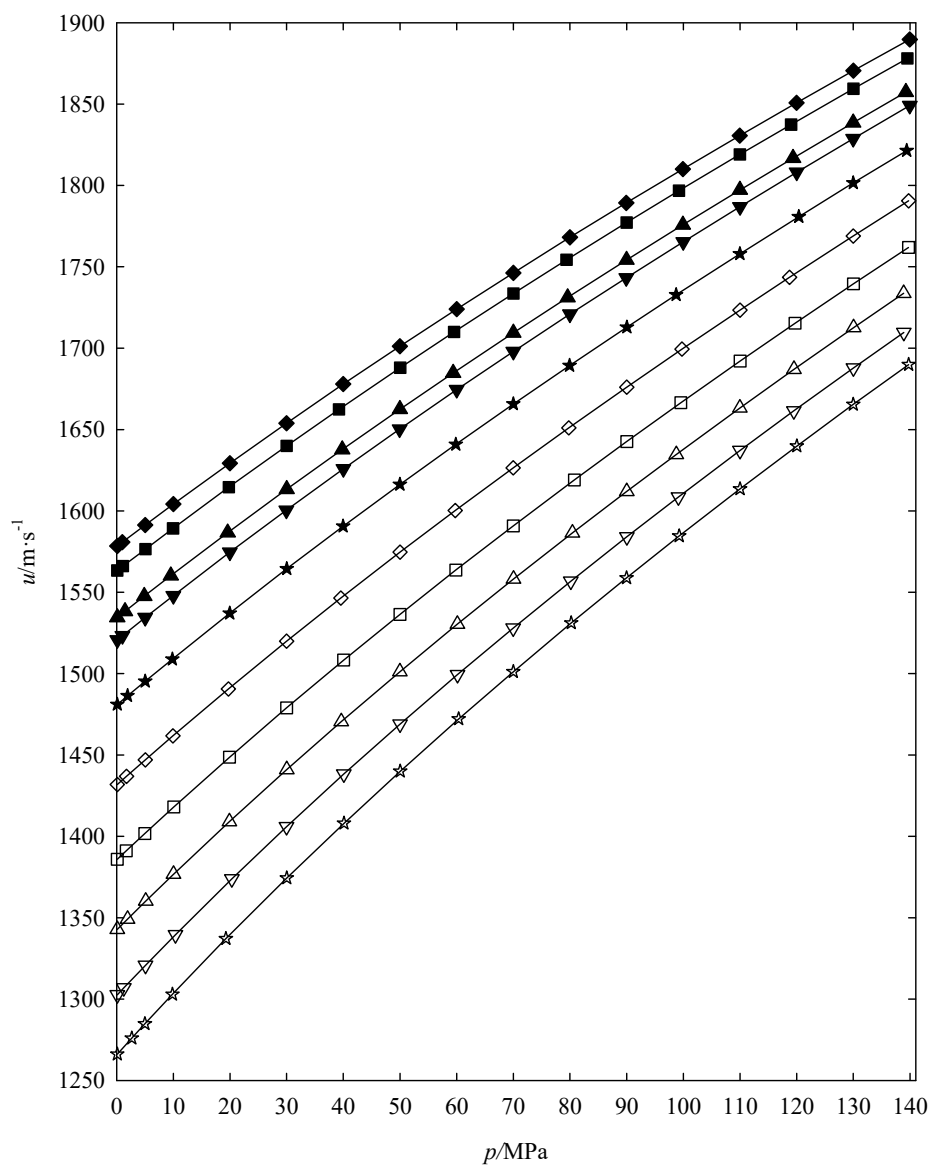


Fig. S-7. Plot of speed of sound $u / \text{m}\cdot\text{s}^{-1}$ of [OMIM][BF₄] versus pressure p : \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.16 K; \triangle , 373.16 K; ∇ , 393.14 K; \star , 413.14 K; the lines are the best fit lines.

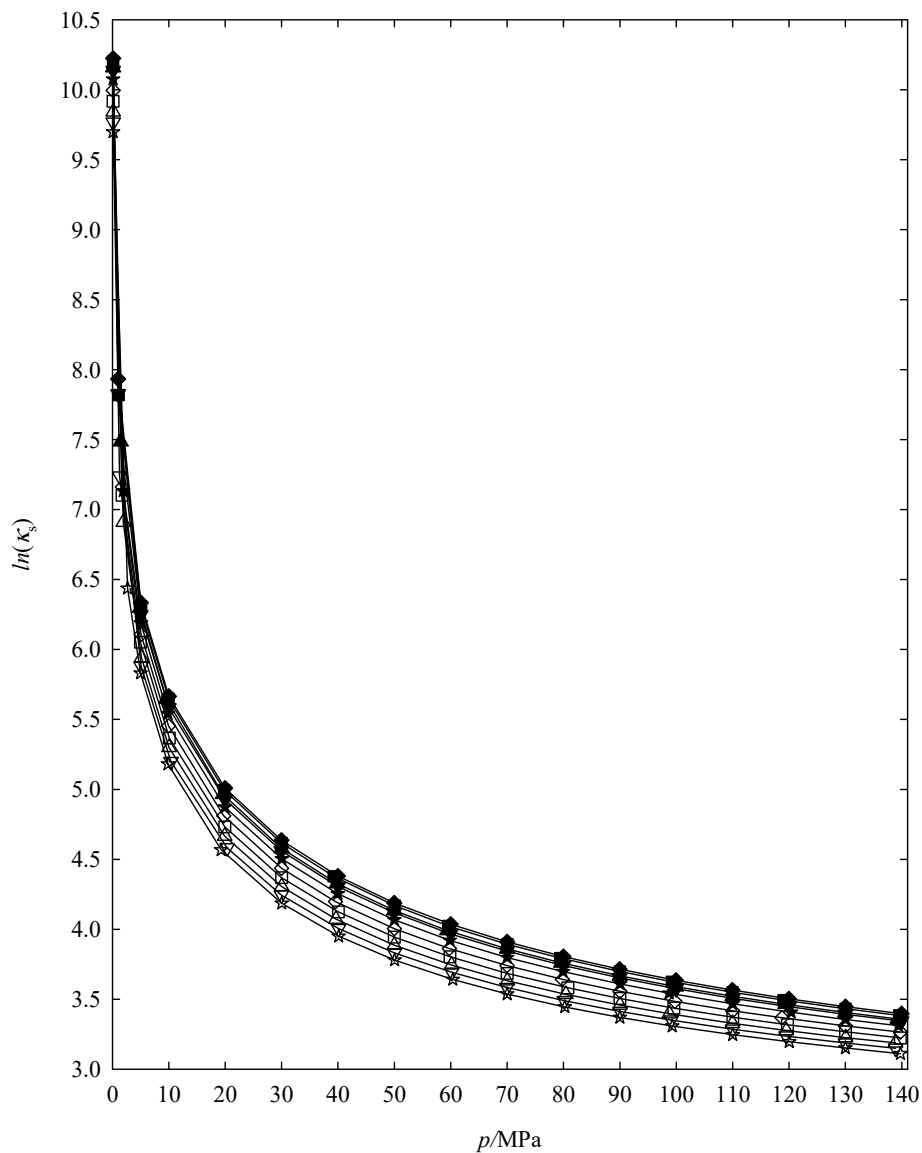


Fig. S-8. Plot of isentropic exponent $\ln(\kappa_s)$ of [OMIM][BF₄] versus pressure p : \blacklozenge , 278.15 K; \blacksquare , 283.15 K; \blacktriangle , 293.15 K; \blacktriangledown , 298.15 K; \star , 313.16 K; \diamond , 333.15 K; \square , 353.16 K; \triangle , 373.16 K; ∇ , 393.14 K; \star , 413.14 K; the lines are the best fit lines.

TABLE S-I. Summary of previous density investigations of [OMIM][BF₄] and the present work

First author	Ref	Year	Method	Properties	Temperature, T / K^a	Pressure, p / MPa	Uncertainty, $\Delta\rho$	F.E.	Purity	IL Source
Gu	7	2002	UPDA	ρ, T	298 and 323	0.099 to 206.94	$\pm 8 \text{ kg}\cdot\text{m}^{-3} (\rho)$	Tait	99%	LP
Harris	8	2006	VTD	ρ, T, η	273.15 to 353.15	0.101 to 224.2	$\pm 0.05 \text{ kg}\cdot\text{m}^{-3} (\rho)$	Tait	H ₂ O cont=54 \pm 10 \cdot 10 ⁻⁶	LP
Gardas	9	2007	VTD	p, ρ, T, η	293.15 to 392.15	0.101 to 10.0	$\pm 0.3 \text{ kg}\cdot\text{m}^{-3} (\rho)$ $\pm 0.025 \text{ MPa} (p)$ $\pm 0.01 \text{ K} (T)$		>99 % H ₂ O cont= 371 ppm	IoLiTec
Sanma med	10	2010	VTD	p, ρ, T, η	283.15 to 323.15	0.101 to 60	$\pm 0.30 \text{ kg}\cdot\text{m}^{-3} (\rho)$ $\pm 0.01 \text{ K} (T)$ $\pm 0.01 \text{ MPa} (p)$		>0.99 mass fr.	SI
Tomida	11	2012	VTD	p, ρ, T, η	293.15 to 353.15	0.101 to 20.0	0.2 % (ρ) 10 mK (T) 0.1 MPa (p)	Tait	>98.5 % w.c.<90 ppm	LP
Hossein	12	2013	S	p, ρ, T, κ_S	313 to 452	0.101 to 10	0.24 % (ρ)			
Roshan	13	2013	S	ρ, T	293.15 to 393.15	1 to 10	0.10426, 0.199222 (ρ)			
Ribeiro	14	2014	GCM	ρ, T, V_m, T_g, p_g	194 and 295	2100 and 0.1				IoLiTec
Safarov	t.w.	2016	VTD	p, ρ, T, η, c_p, u	278.15 to 413.15	0.101 to 140	$\pm(0.1 \text{ to } 0.8) \text{ kg}\cdot\text{m}^{-3} (\rho)$	BRE S	w.c.<40 ppm	SA

^a T , temperature; p , pressure; ρ , density; UPDA, ultrahigh-pressure density apparatus; LP – Laboratory product (synthesis); S, Simulated; VTD, Vibration tube densimeter; η , Viscosity; SI., Solvent Innovation; c_p , heat capacity; u , speed of sound; w.c., water content; κ_S , isentropic exponent; GCM, group contribution model; BRES, Baku–Rostock equation of state; SA, Sigma–Aldrich; t.w., this work.

TABLE S-II. Experimental values of pressure p / MPa , density $\rho / \text{kg}\cdot\text{m}^{-3}$, temperature T / K , together with the calculated values of isothermal compressibility $\kappa_T \cdot 10^6 / \text{MPa}^{-1}$, isobaric thermal expansibility $\alpha_p \cdot 10^6 / \text{K}^{-1}$, difference in isobaric and isochoric heat capacities ($c_p - c_v$) / $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$, thermal pressure coefficient $\gamma / \text{MPa}\cdot\text{K}^{-1}$, internal pressure $p_{\text{int}} / \text{MPa}$, isobaric heat capacity $c_p / \text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$, isochoric heat capacity $c_v / \text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$, speed of sound $u / \text{m}\cdot\text{s}^{-1}$ and isentropic exponent κ_S of [OMIM][BF₄]

p	ρ	T	κ_T	α_p	$c_p - c_v$	γ	p_{int}	c_p	c_v	u	κ_S
0.101	1117.16	278.15	413.3	611.4	225.23	1.4794	411.4	1726.90	1501.67	1578.39	27551.56
1.002	1117.56	278.16	411.8	609.7	224.76	1.4808	410.9	1726.74	1501.99	1580.74	2786.420
5.032	1119.33	278.15	405.1	602.4	222.64	1.4871	408.6	1725.94	1503.29	1591.30	563.221
10.002	1121.48	278.13	397.2	593.7	220.10	1.4948	405.7	1724.92	1504.82	1604.19	288.541
19.968	1125.74	278.15	382.4	577.1	215.23	1.5094	399.9	1722.99	1507.76	1629.30	149.669
29.958	1129.91	278.14	368.6	561.6	210.57	1.5234	393.8	1720.94	1510.37	1653.88	103.179
40.002	1134.00	278.15	355.9	546.9	206.12	1.5368	387.5	1718.86	1512.74	1677.89	79.822
49.985	1137.97	278.15	344.1	533.1	201.89	1.5495	381.0	1716.70	1514.81	1701.20	65.896
60.001	1141.86	278.17	333.1	520.1	197.83	1.5615	374.4	1714.49	1516.66	1723.97	56.567
69.987	1145.64	278.15	322.8	507.8	193.92	1.5731	367.6	1712.09	1518.17	1746.26	49.922

80.002	1149.33	278.15	313.1	496.0	190.15	1.5841	360.6	1709.62	1519.47	1768.08	44.913
89.935	1152.89	278.16	304.2	485.0	186.55	1.5944	353.6	1707.08	1520.53	1789.24	41.040
99.924	1156.38	278.15	295.7	474.4	183.05	1.6043	346.3	1704.37	1521.32	1810.08	37.916
109.953	1159.79	278.15	287.7	464.2	179.65	1.6136	338.9	1701.54	1521.89	1830.61	35.347
119.957	1163.09	278.13	280.1	454.5	176.34	1.6226	331.3	1698.53	1522.20	1850.73	33.210
130.005	1166.30	278.15	272.9	445.2	173.15	1.6310	323.6	1695.50	1522.35	1870.48	31.387
139.953	1169.39	278.15	266.2	436.3	170.06	1.6388	315.9	1692.30	1522.24	1889.72	29.839
0.101	1113.71	283.15	422.5	613.1	226.28	1.4513	410.8	1736.90	1510.62	1563.35	26946.35
1.099	1114.16	283.12	420.7	611.3	225.76	1.4532	410.3	1736.67	1510.90	1566.11	2486.241
5.074	1115.95	283.18	414.0	604.2	223.79	1.4595	408.2	1736.11	1512.31	1576.47	546.542
9.959	1118.13	283.17	405.9	595.7	221.42	1.4676	405.6	1735.25	1513.83	1589.28	283.571
19.809	1122.45	283.16	390.6	579.5	216.84	1.4834	400.2	1733.54	1516.70	1614.54	147.713
29.992	1126.81	283.15	376.1	563.8	212.36	1.4991	394.5	1731.74	1519.38	1639.95	101.049
39.224	1130.67	283.14	363.9	550.4	208.50	1.5128	389.1	1730.07	1521.56	1662.39	79.667
50.024	1135.07	283.14	350.6	535.8	204.22	1.5281	382.6	1728.06	1523.85	1687.97	64.653
59.544	1138.85	283.13	339.8	523.6	200.61	1.5410	376.8	1726.21	1525.60	1709.99	55.926
70.018	1142.89	283.14	328.7	511.0	196.82	1.5547	370.2	1724.12	1527.30	1733.60	49.054
79.392	1146.41	283.15	319.4	500.3	193.57	1.5665	364.1	1722.16	1528.60	1754.28	44.435
89.988	1150.28	283.15	309.5	488.8	190.03	1.5793	357.2	1719.82	1529.79	1777.18	40.367
99.230	1153.56	283.16	301.4	479.2	187.06	1.5900	351.0	1717.70	1530.64	1796.73	37.523
109.987	1157.26	283.16	292.5	468.6	183.72	1.6020	343.6	1715.08	1531.36	1819.07	34.811
119.006	1160.27	283.16	285.5	460.2	181.02	1.6117	337.4	1712.78	1531.76	1837.38	32.909
130.021	1163.84	283.16	277.4	450.3	177.82	1.6231	329.6	1709.84	1532.01	1859.38	30.943
139.540	1166.81	283.16	270.8	442.1	175.14	1.6325	322.7	1707.17	1532.02	1878.04	29.491
0.101	1106.78	293.15	440.8	615.3	227.55	1.3961	409.2	1757.32	1529.77	1534.57	25804.64
1.471	1107.42	293.16	438.2	612.9	226.92	1.3986	408.5	1757.14	1530.23	1538.26	1781.322
4.894	1109.03	293.13	431.8	606.8	225.34	1.4051	407.0	1756.60	1531.26	1547.67	542.810
9.565	1111.20	293.14	423.5	598.7	223.25	1.4136	404.8	1755.97	1532.72	1560.23	282.820
19.598	1115.77	293.15	406.7	582.3	219.00	1.4317	400.1	1754.63	1535.63	1586.66	143.343
30.023	1120.40	293.15	390.7	566.5	214.89	1.4499	395.0	1753.24	1538.35	1613.36	97.149
39.825	1124.63	293.16	376.9	552.7	211.26	1.4664	390.1	1751.94	1540.68	1637.77	75.755
49.979	1128.90	293.16	363.6	539.3	207.72	1.4832	384.8	1750.55	1542.82	1662.45	62.431
59.384	1132.74	293.16	352.2	527.7	204.63	1.4983	379.9	1749.22	1544.59	1684.77	54.146
70.002	1136.95	293.16	340.2	515.4	201.32	1.5150	374.1	1747.66	1546.34	1709.39	47.459
79.597	1140.64	293.15	330.1	504.9	198.48	1.5297	368.8	1746.16	1547.68	1731.15	42.946
89.979	1144.52	293.15	319.8	494.1	195.56	1.5451	363.0	1744.48	1548.93	1754.18	39.140
99.934	1148.11	293.16	310.6	484.4	192.89	1.5595	357.3	1742.82	1549.93	1775.78	36.227
109.976	1151.61	293.15	301.8	475.0	190.31	1.5738	351.4	1741.00	1550.69	1797.17	33.822
119.373	1154.79	293.15	294.1	466.7	188.00	1.5868	345.8	1739.23	1551.23	1816.81	31.933
129.971	1158.24	293.15	285.9	457.8	185.50	1.6012	339.4	1737.13	1551.64	1838.55	30.128
139.266	1161.16	293.15	279.1	450.3	183.38	1.6135	333.7	1735.19	1551.81	1857.28	28.768
0.101	1103.47	298.15	450.0	616.1	227.95	1.3692	408.1	1767.74	1539.79	1520.70	25262.03
1.023	1103.90	298.15	448.1	614.4	227.53	1.3710	407.7	1767.61	1540.09	1523.27	2503.586
5.041	1105.81	298.14	440.4	607.2	225.73	1.3788	406.0	1767.05	1541.32	1534.43	516.463
10.002	1108.13	298.15	431.2	598.6	223.60	1.3883	403.9	1766.43	1542.83	1547.90	265.459
19.985	1112.73	298.13	413.9	582.4	219.55	1.4071	399.5	1765.14	1545.59	1574.61	138.063
29.935	1117.19	298.15	398.1	567.4	215.80	1.4252	395.0	1763.97	1548.17	1600.39	95.600
40.004	1121.59	298.16	383.4	553.4	212.27	1.4432	390.3	1762.78	1550.51	1625.81	74.118

49.923	1125.81	298.15	370.0	540.4	209.02	1.4605	385.5	1761.57	1552.55	1650.26	61.421
60.008	1129.98	298.16	357.4	528.1	205.92	1.4777	380.6	1760.35	1554.43	1674.48	52.802
70.003	1134.00	298.15	345.8	516.7	203.02	1.4944	375.6	1759.05	1556.03	1697.96	46.706
79.985	1137.90	298.13	334.9	506.0	200.29	1.5108	370.4	1757.69	1557.40	1720.91	42.133
89.924	1141.66	298.15	324.8	495.9	197.73	1.5267	365.3	1756.36	1558.64	1743.19	38.578
99.985	1145.36	298.16	315.3	486.3	195.27	1.5425	359.9	1754.93	1559.66	1765.30	35.697
110.006	1148.92	298.15	306.3	477.2	192.93	1.5580	354.5	1753.38	1560.45	1786.92	33.349
120.004	1152.37	298.14	297.9	468.6	190.71	1.5731	349.0	1751.74	1561.04	1808.09	31.393
129.957	1155.68	298.15	290.0	460.4	188.61	1.5879	343.5	1750.08	1561.48	1828.73	29.742
139.954	1158.89	298.15	282.5	452.7	186.59	1.6025	337.8	1748.30	1561.71	1849.13	28.317
0.101	1093.31	313.15	477.8	617.9	228.89	1.2932	404.9	1799.86	1570.96	1481.04	23740.74
1.930	1094.23	313.13	473.7	614.5	228.11	1.2971	404.2	1799.54	1571.44	1486.41	1252.525
5.032	1095.77	313.16	467.1	608.8	226.82	1.3035	403.2	1799.17	1572.35	1495.29	486.857
9.821	1098.14	313.18	457.1	600.4	224.90	1.3134	401.5	1798.56	1573.67	1508.89	254.571
19.940	1103.04	313.18	437.5	583.8	221.12	1.3342	397.9	1797.30	1576.17	1537.09	130.704
30.024	1107.79	313.17	419.7	568.5	217.71	1.3547	394.2	1796.13	1578.42	1564.41	90.308
39.958	1112.35	313.16	403.6	554.7	214.64	1.3744	390.5	1795.06	1580.42	1590.52	70.428
49.979	1116.81	313.16	388.7	541.8	211.80	1.3941	386.6	1794.06	1582.26	1616.20	58.371
59.850	1121.08	313.15	375.1	530.0	209.23	1.4132	382.7	1793.08	1583.85	1640.89	50.434
70.004	1125.34	313.15	362.1	518.7	206.80	1.4326	378.6	1792.12	1585.32	1665.66	44.597
79.915	1129.36	313.15	350.3	508.4	204.61	1.4512	374.5	1791.18	1586.57	1689.29	40.325
90.030	1133.34	313.15	339.1	498.6	202.54	1.4701	370.3	1790.21	1587.67	1712.89	36.930
98.725	1136.66	313.16	330.1	490.6	200.89	1.4861	366.7	1789.38	1588.49	1732.76	34.563
109.978	1140.80	313.16	319.2	480.9	198.90	1.5066	361.8	1788.25	1589.35	1757.98	32.053
120.378	1144.48	313.17	309.7	472.4	197.21	1.5253	357.3	1787.19	1589.98	1780.79	30.147
129.996	1147.76	313.16	301.5	465.1	195.74	1.5426	353.1	1786.12	1590.38	1801.53	28.655
139.395	1150.85	313.16	293.9	458.2	194.40	1.5592	348.9	1785.06	1590.65	1821.43	27.393
0.101	1079.64	333.15	516.5	622.3	231.32	1.2047	401.3	1844.64	1613.32	1431.86	21916.88
1.733	1080.53	333.15	512.3	619.0	230.62	1.2084	400.8	1844.28	1613.66	1436.89	1287.402
5.048	1082.30	333.15	503.9	612.6	229.26	1.2159	400.0	1843.59	1614.33	1447.03	448.985
9.927	1084.89	333.16	492.1	603.6	227.35	1.2267	398.8	1842.65	1615.30	1461.72	233.540
19.736	1089.98	333.15	470.0	586.7	223.84	1.2484	396.2	1840.86	1617.02	1490.63	122.739
29.988	1095.14	333.15	449.1	570.7	220.57	1.2708	393.4	1839.21	1618.64	1519.91	84.378
39.557	1099.81	333.15	431.3	557.0	217.86	1.2915	390.7	1837.83	1619.97	1546.45	66.500
50.011	1104.76	333.16	413.5	543.2	215.21	1.3137	387.7	1836.48	1621.27	1574.65	54.776
59.751	1109.22	333.17	398.3	531.4	213.00	1.3343	384.8	1835.33	1622.33	1600.24	47.537
69.979	1113.74	333.16	383.6	520.0	210.92	1.3558	381.7	1834.17	1623.24	1626.44	42.097
79.790	1117.93	333.16	370.5	509.9	209.13	1.3762	378.7	1833.14	1624.00	1651.00	38.185
90.004	1122.14	333.15	357.8	500.0	207.46	1.3973	375.5	1832.10	1624.63	1676.02	35.015
99.766	1126.01	333.14	346.6	491.2	206.03	1.4174	372.4	1831.15	1625.12	1699.41	32.589
109.994	1129.91	333.14	335.6	482.6	204.69	1.4383	369.2	1830.21	1625.52	1723.41	30.506
118.728	1133.11	333.14	326.7	475.7	203.66	1.4560	366.3	1829.42	1625.76	1743.51	29.009
129.979	1137.06	333.14	316.0	467.4	202.48	1.4788	362.7	1828.43	1625.96	1768.92	27.374
139.759	1140.34	333.15	307.4	460.5	201.57	1.4984	359.4	1827.60	1626.04	1790.57	26.165
0.101	1066.28	353.15	558.0	631.1	236.43	1.1311	399.3	1891.56	1655.14	1385.95	20278.39
1.702	1067.20	353.15	553.1	627.7	235.74	1.1349	399.1	1891.06	1655.32	1391.18	1213.546
4.947	1069.04	353.15	543.5	621.0	234.38	1.1426	398.6	1890.07	1655.69	1401.70	424.606
10.078	1071.92	353.16	529.0	610.8	232.36	1.1548	397.7	1888.59	1656.23	1418.05	213.905

19.928	1077.32	353.16	503.3	592.8	228.85	1.1778	396.0	1885.93	1657.08	1448.68	113.474
30.004	1082.68	353.16	479.7	576.2	225.70	1.2012	394.2	1883.46	1657.76	1478.99	78.944
40.055	1087.84	353.16	458.3	561.1	222.95	1.2241	392.3	1881.22	1658.27	1508.30	61.792
49.978	1092.78	353.15	439.2	547.5	220.55	1.2466	390.3	1879.15	1658.60	1536.42	51.617
59.854	1097.53	353.16	421.8	535.1	218.45	1.2687	388.2	1877.29	1658.84	1563.61	44.829
69.987	1102.23	353.15	405.3	523.4	216.54	1.2912	386.0	1875.47	1658.92	1590.83	39.852
80.761	1107.03	353.14	389.3	511.9	214.77	1.3150	383.6	1873.66	1658.90	1619.04	35.924
90.004	1110.99	353.15	376.6	502.8	213.43	1.3351	381.5	1872.25	1658.81	1642.64	33.299
99.542	1114.93	353.15	364.4	494.0	212.21	1.3559	379.3	1870.84	1658.63	1666.51	31.100
110.030	1119.09	353.16	351.9	485.0	211.04	1.3785	376.8	1869.40	1658.36	1692.11	29.115
119.712	1122.75	353.17	341.1	477.3	210.11	1.3992	374.5	1868.14	1658.04	1715.30	27.591
130.002	1126.48	353.16	330.4	469.6	209.23	1.4212	371.9	1866.83	1657.59	1739.49	26.219
139.720	1129.83	353.16	320.9	462.8	208.53	1.4419	369.5	1865.66	1657.13	1761.89	25.108
0.101	1053.09	373.15	602.5	644.0	243.98	1.0689	398.7	1940.61	1696.62	1342.86	18796.03
1.917	1054.17	373.14	596.0	639.9	243.22	1.0736	398.7	1939.87	1696.64	1349.17	1000.723
5.136	1056.07	373.15	584.9	632.8	241.93	1.0819	398.6	1938.66	1696.72	1360.19	380.364
10.024	1058.92	373.14	568.8	622.5	240.08	1.0945	398.4	1936.81	1696.73	1376.71	200.216
19.898	1064.55	373.15	539.1	603.4	236.73	1.1193	397.8	1933.36	1696.63	1409.03	106.231
30.014	1070.14	373.16	511.9	585.8	233.75	1.1444	397.0	1930.05	1696.31	1441.03	74.054
39.630	1075.28	373.17	488.7	570.7	231.27	1.1679	396.2	1927.09	1695.83	1470.46	58.680
49.974	1080.64	373.16	466.0	555.9	228.92	1.1928	395.1	1924.04	1695.12	1501.18	48.739
60.128	1085.71	373.16	445.9	542.6	226.91	1.2169	394.0	1921.22	1694.30	1530.43	42.298
70.024	1090.48	373.16	427.9	530.7	225.20	1.2402	392.8	1918.60	1693.40	1558.14	37.810
80.421	1095.30	373.17	410.7	519.2	223.63	1.2642	391.4	1916.00	1692.38	1586.48	34.279
90.019	1099.58	373.18	396.0	509.4	222.35	1.2862	390.0	1913.71	1691.36	1611.99	31.740
98.752	1103.34	373.19	383.6	501.0	221.33	1.3061	388.7	1911.71	1690.38	1634.69	29.855
109.976	1107.97	373.17	368.8	491.0	220.16	1.3314	386.9	1909.18	1689.02	1663.27	27.871
119.510	1111.73	373.15	357.1	483.0	219.30	1.3527	385.3	1907.12	1687.82	1687.00	26.477
130.034	1115.70	373.16	345.1	474.9	218.49	1.3760	383.4	1904.99	1686.50	1712.62	25.171
138.874	1118.88	373.16	335.7	468.4	217.90	1.3954	381.8	1903.27	1685.37	1733.66	24.224
0.101	1039.55	393.15	649.2	657.4	251.89	1.0127	398.0	1991.79	1739.90	1302.65	17458.29
1.276	1040.29	393.15	644.3	654.7	251.49	1.0161	398.2	1991.33	1739.84	1306.95	1392.096
5.086	1042.67	393.17	629.1	646.1	250.27	1.0270	398.7	1989.93	1739.66	1320.73	357.517
10.377	1045.93	393.18	609.1	634.7	248.68	1.0421	399.4	1987.95	1739.28	1339.52	180.840
20.336	1051.92	393.15	574.8	615.1	245.99	1.0701	400.4	1984.17	1738.18	1373.90	97.652
29.978	1057.53	393.13	545.4	598.1	243.74	1.0966	401.1	1980.61	1736.87	1405.95	69.747
40.097	1063.23	393.12	517.8	581.9	241.69	1.1237	401.6	1976.98	1735.29	1438.34	54.870
50.015	1068.63	393.13	493.6	567.4	239.95	1.1497	402.0	1973.53	1733.58	1469.03	46.117
60.161	1073.96	393.14	471.1	553.9	238.39	1.1758	402.1	1970.07	1731.68	1499.46	40.140
69.971	1078.92	393.14	451.4	541.9	237.06	1.2005	402.0	1966.76	1729.70	1528.03	36.002
80.150	1083.87	393.13	432.6	530.4	235.83	1.2258	401.8	1963.37	1727.53	1556.86	32.774
90.030	1088.49	393.14	416.0	520.0	234.79	1.2500	401.4	1960.19	1725.39	1584.08	30.334
99.120	1092.57	393.15	401.8	511.1	233.94	1.2718	400.9	1957.32	1723.37	1608.52	28.514
109.998	1097.25	393.13	386.2	501.1	233.02	1.2977	400.2	1953.88	1720.86	1637.10	26.730
119.495	1101.15	393.12	373.5	493.0	232.31	1.3199	399.4	1950.97	1718.66	1661.46	25.435
130.004	1105.26	393.13	360.5	484.5	231.63	1.3441	398.4	1947.87	1716.24	1687.80	24.219
138.906	1108.58	393.14	350.2	477.7	231.11	1.3644	397.5	1945.31	1714.20	1709.64	23.331
0.101	1025.75	413.15	695.5	664.9	256.15	0.9561	394.9	2045.08	1788.93	1266.09	16275.33

2.678	1027.45	413.13	683.3	659.3	255.81	0.9648	395.9	2044.46	1788.65	1276.03	624.612
4.989	1028.97	413.15	672.9	654.4	255.52	0.9724	396.8	2043.99	1788.48	1284.78	340.421
9.857	1032.13	413.19	652.1	644.4	254.95	0.9883	398.5	2042.94	1787.99	1302.91	177.764
19.284	1038.12	413.14	615.2	626.7	253.99	1.0187	401.6	2040.34	1786.36	1337.12	96.275
30.020	1044.71	413.16	578.4	608.5	253.10	1.0520	404.6	2037.32	1784.22	1374.39	65.758
40.114	1050.68	413.18	547.9	593.1	252.41	1.0825	407.2	2034.26	1781.85	1408.05	51.945
50.025	1056.34	413.16	521.0	579.3	251.82	1.1118	409.3	2030.95	1779.13	1439.99	43.797
60.345	1062.02	413.14	495.9	566.0	251.29	1.1414	411.2	2027.36	1776.07	1472.15	38.147
69.986	1067.12	413.14	474.7	554.6	250.87	1.1684	412.7	2023.97	1773.10	1501.16	34.361
80.230	1072.32	413.13	454.1	543.3	250.47	1.1964	414.1	2020.23	1769.77	1531.13	31.331
89.976	1077.08	413.13	436.2	533.3	250.12	1.2225	415.1	2016.65	1766.52	1558.83	29.084
99.285	1081.43	413.12	420.5	524.3	249.81	1.2469	415.8	2013.15	1763.34	1584.63	27.345
110.011	1086.22	413.12	403.8	514.6	249.49	1.2744	416.5	2009.12	1759.64	1613.56	25.702
120.014	1090.47	413.11	389.5	506.1	249.19	1.2995	416.8	2005.32	1756.13	1639.87	24.431
129.986	1094.50	413.13	376.2	498.1	248.93	1.3240	417.0	2001.62	1752.70	1665.45	23.355
139.746	1098.25	413.15	364.1	490.6	248.68	1.3475	417.0	1998.02	1749.34	1689.92	22.447

^a Standard uncertainties u are $u(T) = 0.015$ K, $u(p) = 0.1$ MPa for $p < 100$ MPa, $u(p) = 0.25$ MPa for $p > 100$ MPa, and the combined expanded uncertainty U_c is $U_c(\rho) = 0.1$ kg·m⁻³ for $T > 353$ K, $U_c(\rho) = 0.5$ kg·m⁻³ for 313.15 K $< T < 353$ K, $U_c(\rho) = 0.8$ kg·m⁻³ for $T < 313.15$ K (0.95 level of confidence).

TABLE S-III. Values of the coefficients a_i , b_i and c_i in Eqs. (3–5); standard uncertainties: $\Delta\rho/\rho = 100(\rho_{\text{exp}} - \rho_{\text{cal}})/\rho_{\text{exp}} = \pm 0.011$ %, $\Delta\rho_{\text{abs}} = 0.12$ kg m⁻³

$a_1 = -4.4263437315$	$b_0 = -1264.569925$	$c_0 = 618.5768817$
$a_2 = 0.016257512586$	$b_1 = 12.737638971839$	$c_1 = -5.517724532102$
$a_3 = -0.15794791072 \times 10^{-4}$	$b_2 = -0.03756489737$	$c_2 = 0.0161699715822$
$a_4 = -0.2163681517 \times 10^{-8}$	$b_3 = 0.3709715726 \times 10^{-4}$	$c_3 = -0.156313624062 \times 10^{-4}$

TABLE S-IV. Values of the coefficients d_{ij} in Eq. (10); standard uncertainties: $\Delta c_p/c_p = 100(c_{p \text{ cal}} - c_{p \text{ eq}})/c_{p \text{ eq}} = \pm 0.0164$ %

$d_{00} = 406.742631$	$d_{12} = -0.1051136211 \times 10^{-2}$	$d_{30} = -0.2356469685 \times 10^{-3}$
$d_{01} = 0.2680877455$	$d_{13} = 0.1026992215 \times 10^{-5}$	$d_{31} = 0.2359058760 \times 10^{-5}$
$d_{02} = 0.3345276570 \times 10^{-2}$	$d_{20} = 0.1197208979$	$d_{32} = -0.7820934158 \times 10^{-8}$
$d_{03} = -0.6151985718 \times 10^{-6}$	$d_{21} = -0.1204270691 \times 10^{-2}$	$d_{33} = 0.8510800030 \times 10^{-11}$
$d_{10} = -39.33643656$	$d_{22} = 0.3962511809 \times 10^{-5}$	
$d_{11} = 0.3536293945$	$d_{23} = -0.4252989417 \times 10^{-8}$	

TABLE S-V. Values of the coefficients e_{ij} in Eq. (11); standard uncertainties: $\Delta c_v/c_v = 100(c_{v \text{ cal}} - c_{v \text{ eq}})/c_{v \text{ eq}} = \pm 0.0583$ %

$e_{00} = 766.1409560$	$e_{12} = -0.3483195788 \times 10^{-3}$	$e_{30} = -0.6019367077 \times 10^{-4}$
$e_{01} = 3.842072608$	$e_{13} = 0.3292693216 \times 10^{-6}$	$e_{31} = 0.6493410902 \times 10^{-6}$
$e_{02} = -0.6399909702 \times 10^{-2}$	$e_{20} = 0.3606368913 \times 10^{-1}$	$e_{32} = -0.2295047815 \times 10^{-8}$
$e_{03} = 0.7473829845 \times 10^{-5}$	$e_{21} = -0.3920784094 \times 10^{-3}$	$e_{33} = 0.2705216425 \times 10^{-11}$
$e_{10} = -0.12.6409594$	$e_{22} = 0.1336155735 \times 10^{-5}$	
$e_{11} = 0.1180559868$	$e_{23} = -0.1481146741 \times 10^{-8}$	

TABLE S-VI. Values of the coefficients f_{ij} in Eq. (12); standard uncertainties: $\Delta u/u = 100(u_{\text{cal.}} - u_{\text{eq.}})/u_{\text{cal.}} = \pm 0.0157\%$.

$f_{00} = 3055.70424$	$f_{12} = 0.7085610146 \times 10^{-4}$	$f_{30} = 0.2130258297 \times 10^{-4}$
$f_{01} = -8.321961491$	$f_{13} = -0.6013887533 \times 10^{-7}$	$f_{31} = -0.1605072739 \times 10^{-6}$
$f_{02} = 0.01321000312$	$f_{20} = -0.01314060539$	$f_{32} = 0.4151086310 \times 10^{-9}$
$f_{03} = -0.8603791272 \times 10^{-5}$	$f_{21} = 0.8961532831 \times 10^{-4}$	$f_{33} = -0.1701884673 \times 10^{-12}$
$f_{10} = 3.520584212$	$f_{22} = -0.2280934079 \times 10^{-6}$	
$f_{11} = -0.01826157289$	$f_{23} = 0.1054694514 \times 10^{-9}$	