

# Influence of Temperature on Thermodynamic Properties of Methyl *t*-Butyl Ether (MTBE) + Gasoline Additives

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**Abstract** The densities and sound speeds of binary mixtures of methyl *tert*-butyl ether (MTBE)+(benzene, toluene, ethylbenzene, isooctane, *tert*-butyl alcohol) have been measured at temperatures from 288.15 to 323.15 K and at atmospheric pressure over the complete concentration range. The experimental excess volumes and deviations of isentropic compressibility were calculated. The deviation of isentropic compressibility data have been analyzed in terms of different theoretical models; adequate agreement between the experimental and predicted values is obtained. The data from this study improve the data situation related to gasoline additives and help to understand the MTBE volumetric and acoustic behavior for various chemical systems.

**Keywords** Densities · Sound speeds · Isentropic compressibilities · Model · MTBE · Temperature

## 1 Introduction

Methyl *tert*-butyl ether (MTBE) is the most widely used oxygenated fuel additive employed to improve the combustion efficiency of gasoline and increase its octane rating. Due to its high solubility in water, low Henry's law constant, low partition coefficient of octanol–water, and slow biodegradability, MTBE is relatively stable and

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recalcitrant to many other gasoline compounds in aqueous media [1–3]. Applied processes such as those in the chemical industry or the purification of water are dependent on physical properties of mixtures and their temperature and pressure dependences. A knowledge of the thermodynamic properties of fuel oxygenates such as MTBE with different compounds contained in a typical gasoline is of practical interest to the petrochemical industry. Moreover, this information is useful to develop removal units for spilled MTBE in groundwater. In accordance with that, in the last few years, considerable effort has been applied in the field of thermodynamic properties where a scarcity of data is observed in the open literature for mixtures involved in commercial gasoline. Such properties are strongly dependent on the molecular structure, hydrogen-bond potency of hydroxyl groups, chain length, and isomeric structures.

As a part of an extensive study related to theoretical and experimental analysis of mixtures containing oxygenated and gasoline compounds, we present in this paper the temperature dependences of the density and sound speeds of the binary mixtures of MTBE + (benzene, toluene, ethylbenzene, iso-octane, and *tert*-butyl alcohol (TBA)) at temperatures from 288.15 to 323.15 K and at atmospheric pressure as a function of composition. Due to the expense of experimental measurements such as described here and since current process design is strongly computer oriented, consideration was also given to the performance of several theoretical models. Despite the importance of computation in chemical processes, the theoretical models available in the literature are not always reliable and may have a limited range of application. Our purpose here is to analyze the dependence of the density and isentropic compressibility of mixtures on composition and molecular structure, in order to provide a better understanding concerning the factors which contribute to the behavior of MTBE and other gasoline additives. This category includes slightly polar molecules, aliphatic hydrocarbons and different aryl compounds. The molecular interactions in these systems are complex, and volumetric and isentropic compressibility data provide valuable information for understanding their behavior and structure, as well as valuable input for testing various models for prediction of solution properties. Different schemes [4–6] have been applied for predictions of isentropic compressibility, with the obtained results being analyzed and discussed. Attending to the deviations of computed data, we arrive at the conclusion that the application of the free length theory model with simple mixing laws provides accurate results, despite the highly non-ideal behavior of the mixtures and the influence of temperature.

## 2 Experimental

All chemical solvents used in the preparation of samples were of Merck quality with a purity better than 99.5%. The pure components were stored in glass containers protected from sunlight and at constant humidity and temperature. In order to reduce the error in the composition determination, the vapor space in the vessels was minimized during sample preparation. Each vial was weighed with a precision ( $\pm 2 \times 10^{-5}$  g) balance (GRAM-VXI Series Analytical Balance), with the complete composition range of the binary mixtures being covered. The uncertainty in mole fraction was estimated to be no larger than  $\pm 5 \times 10^{-4}$ . The sound speeds and densities were measured with

**Table 1** Densities ( $\rho$ ) and sound speeds ( $u$ ) of pure components at 298.15 K

Component	$\rho$ (g · cm $^{-3}$ )		$u$ (m · s $^{-1}$ )	
	Exptl.	Lit.	Exptl.	Lit.
MTBE	0.734406	0.73529 [9]	1036.94	1035 [12]
Isooctane	0.687749	0.68762 [9]	1082.20	1083 [13]
Ethylbenzene	0.862459	0.86244 [10]	1318.36	1318 [14]
Benzene	0.873520	0.87356 [10]	1298.27	1299 [14]
Toluene	0.862173	0.86214 [10]	1303.44	1304 [14]
<i>tert</i> -Butyl alcohol (303.15 K)	0.775212	0.77572 [11]	1099.02	1104.8 [15]

an Anton Paar DSA-5000 device with a precision of  $\pm 1$  m · s $^{-1}$  and  $\pm 10^{-5}$  g · cm $^{-3}$ . Calibration of the apparatus was performed periodically, in accordance with technical specifications, using Millipore quality water (resistivity, 18.2 M $\Omega$  cm) and ambient air. More details about techniques and procedure in our laboratory could be obtained from previous papers [7,8]. The measured properties of the pure compounds, as well as open literature data are reported in Table 1.

### 3 Data Procedure

#### 3.1 Correlation of Derived Magnitudes

The corresponding derived magnitudes are presented in Table 2 and were computed from the following equation:

$$\delta Q = Q - \sum_{i=1}^N x_i Q_i \quad (1)$$

In this equation,  $\delta Q$  means the variation of a property  $Q$  ( $V^E$ , excess molar volumes and  $\delta \kappa_S$ , changes of isentropic compressibilities calculated by the Laplace–Newton equation from the density and ultrasonic velocity),  $Q_i$  is the pure component  $i$  property (mixing molar volume or mixing isentropic compressibility),  $x_i$  is the mole fraction, and  $N$  is the number of components in the mixture. Plots of the experimental excess molar volumes and deviations of isentropic compressibility for the binary mixtures of MTBE + (benzene, toluene, ethylbenzene, isoctane, and TBA) are shown in Figs. 1 and 2 at 288.15, 303.15, and 323.15 K. From the experimental values, the corresponding derived properties (excess molar volumes and change of isentropic compressibilities) were fitted with a temperature-dependent Redlich–Kister [16] type polynomial and plotted in Figs. 1 and 2.

**Table 2** Densities, sound speeds, isentropic compressibilities, and derived properties on mixing for MTBE + (benzene, toluene, ethylbenzene, isooctane and *tert*-butyl alcohol) in the range from 288.15 to 323.15 K

$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$\nu^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )	$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$\nu^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )
MTBE + benzene											
288.15 K											
0.000	0.884183	1345.47	624.755	0.000	0.000	0.000	0.881521	1333.44	638.000	0.000	0.000
0.052	0.874712	1328.39	647.864	-4.028	-0.012	0.052	0.872067	1316.51	661.610	-4.370	-0.014
0.111	0.864515	1309.49	674.564	-7.887	-0.034	0.111	0.861888	1297.53	689.151	-8.336	-0.038
0.202	0.849416	1281.74	716.605	-13.195	-0.064	0.202	0.846799	1269.58	732.655	-13.651	-0.069
0.303	0.833719	1252.45	764.644	-17.541	-0.100	0.303	0.831129	1240.48	781.901	-18.416	-0.108
0.397	0.819912	1226.48	810.796	-19.879	-0.119	0.397	0.817328	1214.42	829.594	-20.720	-0.128
0.500	0.805496	1199.09	863.442	-20.864	-0.140	0.500	0.802920	1187.15	883.724	-21.886	-0.149
0.596	0.792712	1174.77	914.069	-20.052	-0.139	0.596	0.790137	1163.01	935.687	-21.284	-0.148
0.698	0.779712	1149.42	970.752	-16.472	-0.122	0.698	0.777135	1137.71	994.124	-17.600	-0.131
0.791	0.768503	1128.20	1022.309	-13.276	-0.108	0.791	0.765921	1116.36	1047.629	-13.958	-0.115
0.902	0.755682	1103.02	1087.662	-5.160	-0.052	0.902	0.753094	1091.23	1115.111	-5.490	-0.056
0.950	0.750294	1092.38	1116.917	-1.116	-0.031	0.950	0.747701	1080.62	1145.318	-1.277	-0.033
1.000	0.744861	1083.38	1143.834	0.000	0.000	1.000	0.742259	1071.61	1173.197	0.000	0.000
290.65 K											
0.000	0.878856	1321.59	651.462	0.000	0.000	0.000	0.876190	1309.88	665.179	0.000	0.000
0.052	0.869419	1304.78	675.610	-4.693	-0.016	0.052	0.866766	1293.02	690.061	-4.867	-0.017
0.111	0.859259	1285.89	703.831	-8.950	-0.042	0.111	0.856624	1274.21	718.998	-9.429	-0.046
0.202	0.844190	1257.97	748.547	-14.558	-0.075	0.202	0.841573	1246.34	764.954	-15.380	-0.081
0.303	0.828533	1228.93	799.164	-19.616	-0.116	0.303	0.825932	1217.35	817.005	-20.755	-0.125
0.397	0.814742	1202.89	848.258	-22.059	-0.138	0.397	0.812151	1191.34	867.545	-23.373	-0.147
0.500	0.800338	1175.60	904.081	-23.235	-0.159	0.500	0.797750	1164.04	925.119	-24.591	-0.169
0.596	0.787557	1151.40	957.780	-22.481	-0.157	0.596	0.784866	1139.79	980.617	-23.702	-0.167
0.698	0.774552	1126.17	1017.985	-18.714	-0.138	0.698	0.771959	1114.60	1042.720	-19.813	-0.146
0.791	0.763334	1104.76	1073.370	-14.728	-0.121	0.791	0.760733	1093.14	1100.059	-15.489	-0.127
0.902	0.750497	1079.57	1143.272	-5.659	-0.059	0.902	0.747886	1067.87	1172.540	-5.753	-0.062
0.950	0.745100	1068.97	1174.504	-1.222	-0.035	0.950	0.742485	1057.24	1204.939	-0.992	-0.036
1.000	0.739654	1060.05	1203.147	0.000	0.000	1.000	0.737036	1048.48	1234.216	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.873520	1298.27	298.15K	679.199	0.000	0.000	0.870847	1286.68	693.613	0.000	0.000
0.052	0.864111	1281.34	704.858	-5.037	-0.019	0.052	0.861451	1269.67	720.092	-5.204	-0.021
0.111	0.853986	1262.58	734.567	-9.894	-0.050	0.111	0.851345	1250.99	750.562	-10.410	-0.054
0.202	0.838954	1234.76	781.802	-16.219	-0.088	0.202	0.836329	1223.24	799.097	-17.157	-0.095
0.303	0.823323	1205.79	835.384	-21.892	-0.133	0.303	0.820710	1194.30	854.247	-23.167	-0.142
0.397	0.809552	1179.81	887.424	-24.703	-0.157	0.397	0.806945	1168.34	907.857	-26.170	-0.167
0.500	0.795155	1152.52	946.785	-26.007	-0.179	0.500	0.792548	1141.04	969.109	-27.532	-0.189
0.596	0.782366	1128.18	1004.230	-24.910	-0.176	0.596	0.779760	1116.71	1028.391	-26.410	-0.186
0.698	0.769356	1103.03	1068.312	-20.896	-0.155	0.698	0.766742	1091.50	1094.721	-22.079	-0.163
0.791	0.758126	1081.51	1127.710	-16.201	-0.134	0.791	0.755506	1069.97	1156.163	-17.099	-0.140
0.902	0.745267	1056.19	1202.829	-5.826	-0.065	0.902	0.742638	1044.66	1233.880	-6.206	-0.068
0.950	0.739860	1045.49	1236.547	-0.626	-0.038	0.950	0.737224	1033.85	1269.070	-0.451	-0.039
1.000	0.734406	1036.94	1266.358	0.000	0.000	1.000	0.731766	1025.42	1299.643	0.000	0.000
0.000	0.868172	1275.13	708.411	0.000	0.000	0.865490	1263.59	723.645	0.000	0.000	0.000
0.052	0.858785	1258.05	735.732	-5.394	-0.022	0.052	0.856117	1246.47	751.802	-5.632	-0.024
0.111	0.848697	1239.45	766.989	-10.976	-0.058	0.111	0.846045	1227.96	783.859	-11.623	-0.063
0.202	0.833698	1211.73	816.920	-18.127	-0.102	0.202	0.831061	1200.28	835.222	-19.216	-0.109
0.303	0.818089	1182.82	873.700	-24.500	-0.150	0.303	0.815461	1171.41	893.674	-25.989	-0.160
0.397	0.804330	1156.89	928.927	-27.730	-0.177	0.397	0.801707	1145.50	950.592	-29.447	-0.187
0.500	0.789936	1129.61	992.090	-29.221	-0.199	0.500	0.787314	1118.22	1015.775	-31.040	-0.210
0.596	0.777144	1105.25	1053.362	-28.003	-0.196	0.596	0.774518	1093.82	1079.137	-29.703	-0.206
0.698	0.764119	1080.03	1121.934	-23.449	-0.171	0.698	0.761485	1068.61	1150.006	-24.954	-0.180
0.791	0.752877	1058.49	1185.502	-18.82	-0.147	0.791	0.750234	1047.06	1215.794	-19.381	-0.154
0.902	0.739994	1033.16	1266.009	-6.677	-0.072	0.902	0.737340	1021.69	1299.254	-7.188	-0.075
0.950	0.734576	1022.32	1302.535	-0.544	-0.041	0.950	0.731914	1010.86	1337.082	-0.751	-0.043
1.000	0.729112	1013.90	1334.183	0.000	0.000	1.000	0.726444	1002.41	1369.957	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.862805	1252.08	308.15K	0.000	0.000	0.000	0.860118	1240.69	755.293	0.000	0.000
0.052	0.853440	1234.93	739.304	-5.886	-0.026	0.052	0.850759	1223.50	785.209	-6.148	-0.027
0.111	0.843388	1216.51	801.201	-12.307	-0.067	0.111	0.840726	1205.19	818.907	-13.061	-0.072
0.202	0.828417	1188.88	854.034	-20.372	-0.116	0.202	0.825767	1177.52	873.385	-21.509	-0.123
0.303	0.812827	1160.04	914.231	-27.548	-0.169	0.303	0.810187	1148.77	935.295	-29.217	-0.179
0.397	0.799075	1134.12	972.959	-31.185	-0.198	0.397	0.796438	1122.81	995.945	-33.010	-0.209
0.500	0.784683	1106.86	1040.208	-32.911	-0.221	0.500	0.782044	1095.54	1065.399	-34.829	-0.233
0.596	0.771880	1082.43	1105.734	-31.454	-0.216	0.596	0.769234	1071.17	1132.986	-33.444	-0.227
0.698	0.758841	1057.23	1178.990	-26.495	-0.189	0.698	0.756187	1045.96	1208.762	-28.241	-0.199
0.791	0.747582	1035.66	1247.116	-20.568	-0.161	0.791	0.744918	1024.30	1279.491	-21.783	-0.169
0.902	0.734673	1010.28	1333.590	-7.708	-0.079	0.902	0.731995	998.90	1369.140	-8.200	-0.083
0.950	0.729241	999.43	1372.853	-0.870	-0.045	0.950	0.726556	988.05	1409.850	-0.994	-0.048
1.000	0.723763	990.99	1406.906	0.000	0.000	1.000	0.721069	979.62	1445.133	0.000	0.000
0.000	0.857425	1229.29	771.783	0.000	0.000	0.000	0.854730	1217.94	788.713	0.000	0.000
0.052	0.848070	1212.02	802.692	-6.385	-0.029	0.052	0.845378	1200.62	820.612	-6.667	-0.030
0.111	0.838056	1193.81	837.253	-13.819	-0.077	0.111	0.835381	1182.49	856.092	-14.614	-0.081
0.202	0.823111	1166.26	893.204	-22.938	-0.131	0.202	0.820447	1154.96	913.725	-24.270	-0.138
0.303	0.807533	1137.44	957.156	-30.977	-0.188	0.303	0.804877	1126.17	979.631	-32.810	-0.198
0.397	0.793792	1111.53	1019.649	-35.122	-0.220	0.397	0.791135	1100.35	1043.969	-37.383	-0.231
0.500	0.779391	1084.24	1091.425	-37.049	-0.244	0.500	0.776733	1073.05	1118.120	-39.448	-0.256
0.596	0.766575	1059.84	1161.354	-35.578	-0.238	0.596	0.763908	1048.57	1190.595	-37.766	-0.249
0.698	0.753517	1034.60	1239.830	-30.080	-0.208	0.698	0.750840	1023.31	1271.857	-31.970	-0.218
0.791	0.742240	1012.99	1312.941	-23.429	-0.177	0.791	0.739550	1001.69	1347.615	-24.940	-0.184
0.902	0.729301	987.61	1405.796	-9.233	-0.088	0.902	0.726593	976.23	1444.124	-9.771	-0.091
0.950	0.723852	976.70	1448.198	-1.478	-0.050	0.950	0.721138	965.31	1488.154	-1.569	-0.052
1.000	0.718357	968.16	1485.133	0.000	0.000	1.000	0.715636	956.80	1526.390	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.852032	1206.70	318.15K	0.000	0.000	0.000	0.849331	1195.55	823.735	0.000	0.000
0.052	0.842684	1189.38	838.869	-7.037	-0.032	0.052	0.840006	1178.42	857.270	-7.748	-0.036
0.111	0.832703	1171.29	875.349	-15.472	-0.086	0.111	0.830019	1160.14	895.140	-16.364	-0.091
0.202	0.817778	1143.77	934.732	-25.683	-0.146	0.202	0.815102	1132.63	956.339	-27.196	-0.154
0.303	0.802213	1115.03	1002.622	-34.789	-0.209	0.303	0.799541	1103.90	1026.360	-36.866	-0.219
0.397	0.788472	1089.16	1069.130	-39.553	-0.243	0.397	0.785800	1078.07	1094.949	-42.043	-0.255
0.500	0.774062	1061.85	1145.771	-41.738	-0.268	0.500	0.771341	1050.37	1175.084	-43.494	-0.275
0.596	0.761226	1037.37	1220.728	-39.999	-0.260	0.596	0.758536	1026.21	1251.847	-42.512	-0.272
0.698	0.748147	1012.13	1304.790	-33.989	-0.227	0.698	0.745444	1000.95	1338.937	-36.205	-0.238
0.791	0.736847	990.48	1383.347	-26.513	-0.192	0.791	0.734130	979.25	1420.496	-28.217	-0.201
0.902	0.723870	964.92	1483.737	-10.251	-0.095	0.902	0.721133	953.72	1524.554	-11.230	-0.099
0.950	0.718407	954.05	1529.281	-1.763	-0.054	0.950	0.715663	942.80	1571.999	-2.138	-0.056
1.000	0.712897	945.54	1568.966	0.000	0.000	1.000	0.710141	934.24	1613.387	0.000	0.000
0.000	0.846641	1184.63	841.657	0.000	0.000						
0.052	0.837364	1168.00	875.387	-9.025	-0.043						
0.111	0.827342	1149.19	915.232	-17.325	-0.095						
0.202	0.812432	1121.71	978.254	-28.903	-0.162						
0.303	0.796876	1093.00	1050.434	-39.257	-0.230						
0.397	0.783138	1067.23	1121.103	-44.986	-0.269						
0.500	0.768725	1040.03	1202.644	-47.941	-0.297						
0.596	0.755841	1015.19	1283.734	-45.336	-0.284						
0.698	0.742756	990.11	1373.368	-39.367	-0.251						
0.791	0.731411	968.17	1458.597	-30.332	-0.209						
0.902	0.718400	942.69	1566.375	-12.731	-0.105						
0.950	0.712917	931.73	1615.775	-3.053	-0.059						
1.000	0.707381	922.97	1659.478	0.000	0.000						

**Table 2** continued

$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )	$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )
MTBE+toluene											
0.000	0.871457	1347.50	631.970	0.000	0.000	0.000	0.869144	1336.32	644.299	0.000	0.000
0.053	0.864558	1332.90	651.045	-8.295	-0.077	0.053	0.862236	1321.86	663.748	-8.831	-0.080
0.116	0.856488	1315.92	674.248	-17.055	-0.154	0.116	0.854153	1304.85	687.612	-17.995	-0.158
0.199	0.845884	1295.15	704.773	-29.007	-0.250	0.199	0.845533	1284.23	718.807	-30.690	-0.257
0.301	0.832848	1268.12	746.644	-39.579	-0.343	0.301	0.830472	1257.36	761.650	-42.035	-0.353
0.371	0.824068	1249.47	777.294	-44.686	-0.399	0.371	0.821675	1238.54	793.377	-47.255	-0.410
0.463	0.812346	1225.78	819.283	-49.877	-0.427	0.463	0.809929	1214.99	836.388	-52.994	-0.439
0.610	0.793998	1186.33	894.890	-49.478	-0.450	0.610	0.791542	1175.57	914.174	-52.918	-0.463
0.688	0.784329	1165.98	937.820	-46.129	-0.426	0.688	0.781848	1155.02	958.735	-49.256	-0.438
0.797	0.770893	1137.29	1003.031	-36.847	-0.370	0.797	0.768289	1126.57	1025.555	-40.226	-0.380
0.902	0.757810	1108.52	1073.872	-19.592	-0.263	0.902	0.755262	1098.16	1097.921	-23.230	-0.270
0.943	0.752561	1097.53	1103.127	-11.491	-0.188	0.943	0.750000	1086.78	1128.900	-14.109	-0.195
1.000	0.744861	1083.38	1143.834	0.000	0.000	1.000	0.742259	1071.61	1173.197	0.000	0.000
295.65 K											
0.000	0.866823	1325.34	656.773	0.000	0.000	0.000	0.864500	1314.33	669.617	0.000	0.000
0.053	0.859905	1310.91	676.712	-9.275	-0.082	0.053	0.857569	1299.86	690.141	-9.665	-0.083
0.116	0.851805	1293.82	701.313	-18.793	-0.162	0.116	0.849458	1282.76	715.430	-19.633	-0.166
0.199	0.841167	1273.24	733.326	-32.120	-0.263	0.199	0.838799	1262.16	748.365	-33.551	-0.270
0.301	0.828083	1246.41	777.328	-44.098	-0.361	0.301	0.825688	1235.43	793.501	-46.260	-0.370
0.371	0.819270	1227.54	810.031	-49.562	-0.420	0.371	0.816857	1216.47	827.277	-51.925	-0.430
0.463	0.807497	1203.94	854.377	-55.577	-0.449	0.463	0.805058	1192.95	872.827	-58.415	-0.460
0.610	0.789068	1164.65	934.318	-55.914	-0.473	0.610	0.786387	1153.62	955.273	-58.926	-0.484
0.688	0.779352	1143.93	980.545	-51.938	-0.448	0.688	0.776847	1132.78	1003.167	-54.691	-0.458
0.797	0.765757	1115.72	1049.056	-43.125	-0.388	0.797	0.763216	1104.90	1073.264	-46.284	-0.397
0.902	0.752693	1087.37	1123.641	-25.740	-0.275	0.902	0.750116	1076.72	1149.916	-28.740	-0.281
0.943	0.747415	1075.87	1155.896	-16.066	-0.198	0.943	0.744822	1064.76	1184.252	-17.738	-0.201
1.000	0.739654	1060.05	1203.147	0.000	0.000	1.000	0.737036	1048.48	1234.216	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.862173	1303.44	298.15K	682.690	0.000	0.000	0.859845	1292.64	696.025	0.000	0.000
0.053	0.855229	1288.91	703.837	-10.061	-0.085	0.053	0.852386	1278.06	717.805	-10.495	-0.087
0.116	0.847105	1271.77	729.870	-20.476	-0.170	0.116	0.844749	1260.83	744.662	-21.332	-0.175
0.199	0.836426	1251.18	763.718	-35.064	-0.277	0.199	0.834049	1240.22	779.491	-36.594	-0.283
0.301	0.823289	1224.50	810.084	-48.498	-0.379	0.301	0.820886	1213.56	827.170	-50.759	-0.388
0.371	0.814439	1205.49	844.917	-54.437	-0.440	0.371	0.812020	1194.52	863.071	-57.025	-0.451
0.463	0.802616	1181.85	892.005	-61.147	-0.471	0.463	0.800168	1170.79	911.719	-64.013	-0.483
0.610	0.784100	1142.62	976.843	-62.067	-0.496	0.610	0.781607	1131.60	999.138	-65.283	-0.508
0.688	0.774335	1122.00	1025.854	-58.191	-0.469	0.688	0.771814	1111.37	1048.987	-62.112	-0.480
0.797	0.760667	1093.78	1098.868	-48.950	-0.406	0.797	0.758108	1082.56	1125.550	-51.501	-0.415
0.902	0.747528	1065.70	1177.884	-31.038	-0.287	0.902	0.744931	1054.44	1207.370	-32.875	-0.293
0.943	0.742221	1053.45	1214.057	-18.987	-0.206	0.943	0.739606	1042.06	1245.128	-20.062	-0.210
1.000	0.734406	1036.94	1266.358	0.000	0.000	1.000	0.731766	1025.42	1299.643	0.000	0.000
0.000	0.857513	1281.88	709.683	0.000	0.000	0.855175	1271.16	723.677	0.000	0.000	0.000
0.053	0.850544	1267.26	732.102	-10.973	-0.090	0.053	0.848195	1256.52	746.733	-11.500	-0.092
0.116	0.842388	1249.95	759.806	-22.267	-0.179	0.116	0.840022	1239.11	775.335	-23.256	-0.184
0.199	0.831668	1229.31	795.659	-38.237	-0.290	0.199	0.829282	1218.39	812.316	-39.906	-0.298
0.301	0.818477	1202.64	844.738	-53.142	-0.398	0.301	0.816062	1191.74	862.807	-55.630	-0.408
0.371	0.809592	1183.56	881.766	-59.740	-0.462	0.371	0.807159	1172.63	900.988	-62.596	-0.474
0.463	0.797712	1159.75	932.020	-67.047	-0.495	0.463	0.795249	1148.75	952.897	-70.256	-0.508
0.610	0.779104	1120.64	1022.050	-68.774	-0.521	0.610	0.776592	1109.72	1045.635	-72.475	-0.534
0.688	0.769287	1100.20	1073.911	-65.205	-0.492	0.688	0.766747	1089.04	1099.665	-68.422	-0.505
0.797	0.755539	1071.36	1153.114	-54.237	-0.425	0.797	0.752961	1060.15	1181.661	-57.040	-0.435
0.902	0.742321	1043.10	1238.102	-34.628	-0.299	0.902	0.739700	1031.72	1270.050	-36.311	-0.305
0.943	0.736980	1030.65	1277.385	-21.153	-0.214	0.943	0.734343	1019.26	1310.784	-22.285	-0.219
1.000	0.729112	1013.90	1334.183	0.000	0.000	1.000	0.726444	1002.41	1369.957	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.852838	1260.49	308.15K	737.997	0.000	0.000	0.850494	1249.83	752.709	0.000	0.000
0.053	0.845842	1245.81	761.741	-12.023	-0.094	0.053	0.843486	1235.16	777.098	-12.635	-0.097
0.116	0.837654	1228.31	791.260	-24.274	-0.188	0.116	0.835279	1217.63	807.491	-25.481	-0.193
0.199	0.826891	1207.54	829.371	-41.672	-0.305	0.199	0.824494	1196.72	846.891	-43.541	-0.313
0.301	0.813640	1180.88	881.366	-58.211	-0.418	0.301	0.811214	1170.06	900.427	-60.948	-0.429
0.371	0.804720	1161.75	920.725	-65.579	-0.486	0.371	0.802273	1150.87	941.077	-68.668	-0.499
0.463	0.792780	1137.76	974.420	-73.539	-0.521	0.463	0.790303	1126.82	996.546	-77.021	-0.535
0.610	0.774070	1098.76	1070.075	-76.67	-0.547	0.610	0.771541	1087.74	1095.446	-79.859	-0.561
0.688	0.764201	1077.93	1126.189	-71.778	-0.517	0.688	0.761642	1066.90	1153.458	-75.391	-0.530
0.797	0.750369	1048.99	1211.107	-59.947	-0.445	0.797	0.747769	1037.86	1241.524	-62.982	-0.456
0.902	0.737069	1020.41	1302.994	-38.088	-0.312	0.902	0.734423	1009.13	1337.086	-39.909	-0.319
0.943	0.731692	1008.00	1345.088	-23.639	-0.223	0.943	0.729029	996.73	1380.703	-24.909	-0.228
1.000	0.723763	990.99	1406.906	0.000	0.000	1.000	0.721069	979.62	1445.133	0.000	0.000
0.000	0.848146	1239.22	767.773	0.000	0.000	0.845794	1228.62	783.250	0.000	0.000	0.000
0.053	0.841124	1224.53	792.868	-13.261	-0.099	0.053	0.838757	1213.95	809.026	-13.960	-0.102
0.116	0.832902	1206.97	824.163	-26.763	-0.198	0.116	0.830517	1196.36	841.255	-28.137	-0.203
0.199	0.822092	1186.00	864.789	-45.666	-0.322	0.199	0.819682	1175.32	883.166	-47.894	-0.330
0.301	0.808780	1159.26	920.043	-63.911	-0.440	0.301	0.806341	1148.50	940.198	-67.001	-0.452
0.371	0.799819	1140.11	961.866	-72.199	-0.512	0.371	0.797359	1129.30	983.394	-75.719	-0.525
0.463	0.787815	1115.92	1019.318	-80.868	-0.549	0.463	0.785320	1105.04	1042.791	-84.818	-0.563
0.610	0.769004	1076.74	1121.630	-83.957	-0.576	0.610	0.766457	1065.76	1148.665	-88.134	-0.590
0.688	0.759075	1055.89	1181.620	-79.440	-0.544	0.688	0.756499	1044.90	1210.716	-83.548	-0.559
0.797	0.745157	1026.77	1272.934	-66.507	-0.468	0.797	0.742532	1015.65	1305.560	-69.903	-0.479
0.902	0.731765	997.95	1372.179	-42.362	-0.327	0.902	0.729096	986.80	1408.500	-44.761	-0.334
0.943	0.726353	985.49	1417.581	-26.607	-0.234	0.943	0.723661	974.25	1455.875	-28.099	-0.239
1.000	0.718357	968.16	1485.133	0.000	0.000	1.000	0.715636	956.80	1526.390	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.843437	1218.01	318.15K	0.000	0.000	0.000	0.841075	1207.31	815.695	0.000	0.000
0.053	0.836384	1203.44	825.554	-14.788	-0.104	0.053	0.834008	1192.91	842.586	-15.761	-0.107
0.116	0.828127	1185.76	858.834	-29.578	-0.209	0.116	0.825730	1175.18	876.906	-31.254	-0.214
0.199	0.817267	1164.65	902.080	-50.211	-0.338	0.199	0.814847	1154.09	921.392	-52.963	-0.348
0.301	0.803893	1137.76	960.949	-70.211	-0.464	0.301	0.801438	1127.01	982.369	-73.715	-0.476
0.371	0.794887	1118.51	1005.576	-79.359	-0.539	0.371	0.792407	1107.74	1028.433	-83.375	-0.553
0.463	0.782821	1094.20	1066.950	-88.937	-0.579	0.463	0.780310	1083.37	1091.891	-93.441	-0.595
0.610	0.763899	1054.79	1176.609	-92.383	-0.606	0.610	0.761327	1043.82	1205.529	-97.009	-0.622
0.688	0.753908	1033.84	1241.009	-87.508	-0.573	0.688	0.751303	1022.83	1272.266	-91.955	-0.588
0.797	0.739897	1004.57	1339.271	-73.356	-0.491	0.797	0.737246	993.50	1374.206	-77.174	-0.503
0.902	0.726409	975.59	1446.386	-46.829	-0.342	0.902	0.723713	964.40	1485.659	-49.231	-0.351
0.943	0.720958	963.00	1495.676	-29.352	-0.244	0.943	0.718237	951.77	1536.980	-30.877	-0.250
1.000	0.712897	945.54	1568.966	0.000	0.000	1.000	0.710141	934.24	1613.387	0.000	0.000
0.000	0.838706	1196.60	832.707	0.000	0.000						
0.053	0.831624	1182.39	860.105	-16.809	-0.110						
0.116	0.823329	1164.61	895.500	-33.043	-0.220						
0.199	0.812420	1143.50	941.341	-55.810	-0.357						
0.301	0.798979	1116.42	1004.175	-77.684	-0.489						
0.371	0.789920	1097.02	1051.932	-87.682	-0.567						
0.463	0.777787	1072.53	1117.688	-98.132	-0.610						
0.610	0.758745	1032.94	1235.247	-102.049	-0.637						
0.688	0.748686	1011.90	1304.443	-96.786	-0.601						
0.797	0.734592	982.48	1410.283	-81.282	-0.516						
0.902	0.721000	953.28	1526.243	-51.876	-0.357						
0.943	0.715503	940.59	1579.748	-32.540	-0.254						
1.000	0.707381	922.97	1659.478	0.000	0.000						

**Table 2** continued

$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )	$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )
MTBE+ethylbenzene											
0.000	0.871245	1360.73	288.15K	619.892	0.000	0.000	0.869052	1349.91	631.458	0.000	0.000
0.046	0.866075	1348.32	635.124	-8.867	-0.068	0.046	0.863868	1337.57	647.023	-9.354	-0.070
0.106	0.859155	1334.44	653.628	-22.045	-0.144	0.106	0.856925	1323.37	666.338	-22.796	-0.147
0.212	0.846925	1307.22	690.968	-39.884	-0.262	0.212	0.844671	1296.35	704.479	-41.708	-0.270
0.299	0.836536	1284.60	724.402	-52.383	-0.342	0.299	0.834249	1273.70	738.873	-54.807	-0.351
0.402	0.823953	1256.66	768.532	-62.086	-0.388	0.402	0.821631	1245.62	784.426	-64.916	-0.399
0.503	0.812763	1231.37	811.445	-66.633	-0.425	0.503	0.810408	1220.15	828.838	-69.576	-0.437
0.600	0.799067	1201.33	867.146	-67.169	-0.416	0.600	0.796665	1190.06	886.312	-70.250	-0.428
0.701	0.785930	1171.87	926.525	-60.436	-0.372	0.701	0.783488	1160.52	947.681	-63.314	-0.384
0.822	0.769744	1136.22	1006.303	-44.163	-0.280	0.822	0.767243	1124.48	1030.774	-45.884	-0.289
0.899	0.759058	1112.67	1064.124	-26.983	-0.178	0.899	0.756516	1100.72	1091.009	-27.670	-0.184
0.948	0.752102	1097.35	1104.162	-12.313	-0.072	0.948	0.749532	1085.43	1132.416	-12.492	-0.075
1.000	0.744861	1083.38	1143.834	0.000	0.000	1.000	0.742259	1071.61	1173.197	0.000	0.000
0.000	0.866856	1339.40	293.15K	643.032	0.000	0.000	0.864660	1328.86	654.932	0.000	0.000
0.046	0.861653	1326.80	659.260	-9.535	-0.071	0.046	0.859445	1316.32	671.520	-10.057	-0.073
0.106	0.854698	1312.72	678.958	-23.705	-0.151	0.106	0.852469	1301.98	692.011	-24.594	-0.155
0.212	0.842406	1285.46	718.392	-43.260	-0.277	0.212	0.840144	1274.76	732.469	-45.142	-0.284
0.299	0.831951	1262.79	753.772	-56.985	-0.359	0.299	0.829658	1251.98	768.964	-59.433	-0.369
0.402	0.819300	1234.63	800.725	-67.582	-0.410	0.402	0.816970	1223.67	817.458	-70.458	-0.422
0.503	0.808048	1209.17	846.424	-72.619	-0.450	0.503	0.805684	1198.20	864.523	-75.866	-0.463
0.600	0.794260	1178.96	905.814	-73.349	-0.441	0.600	0.791851	1167.85	925.939	-76.627	-0.454
0.701	0.781040	1149.35	969.219	-66.224	-0.395	0.701	0.778587	1138.14	991.520	-69.253	-0.408
0.822	0.764736	1113.17	1055.275	-48.058	-0.298	0.822	0.762221	1101.82	1080.682	-50.304	-0.307
0.899	0.753964	1089.18	1118.021	-28.758	-0.189	0.899	0.751405	1077.73	1145.792	-30.126	-0.195
0.948	0.746956	1073.85	1160.961	-12.937	-0.078	0.948	0.744369	1062.33	1190.400	-13.567	-0.081
1.000	0.739654	1060.05	1203.147	0.000	0.000	1.000	0.737036	1048.48	1234.216	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.862459	1318.36	298.15K	667.104	0.000	0.000	0.860256	1307.90	679.553	0.000	0.000
0.046	0.857231	1305.99	683.947	-10.721	-0.075	0.046	0.855014	1295.75	696.601	-11.474	-0.077
0.106	0.850237	1291.40	705.242	-25.660	-0.160	0.106	0.848001	1280.88	718.765	-26.805	-0.164
0.212	0.837881	1264.10	746.887	-47.126	-0.293	0.212	0.835613	1253.49	761.646	-49.229	-0.302
0.299	0.827364	1241.21	784.536	-62.013	-0.380	0.299	0.825064	1230.49	800.491	-64.747	-0.391
0.402	0.814636	1212.68	834.726	-73.394	-0.434	0.402	0.812278	1201.50	852.801	-76.148	-0.444
0.503	0.803312	1187.27	883.114	-79.288	-0.476	0.503	0.800937	1176.37	902.223	-82.896	-0.490
0.600	0.789435	1156.76	946.667	-80.056	-0.468	0.600	0.787011	1145.66	968.072	-83.604	-0.481
0.701	0.776124	1126.99	1014.446	-72.490	-0.420	0.701	0.773654	1115.86	1038.087	-75.895	-0.433
0.822	0.759695	1090.49	1106.923	-52.647	-0.316	0.822	0.757162	1079.23	1133.922	-55.220	-0.326
0.899	0.748835	1066.31	1174.483	-31.568	-0.200	0.899	0.746257	1054.93	1204.105	-33.135	-0.206
0.948	0.741772	1050.85	1220.810	-14.256	-0.084	0.948	0.739163	1039.40	1252.260	-15.004	-0.087
1.000	0.734406	1036.94	1266.358	0.000	0.000	1.000	0.731766	1025.42	1299.643	0.000	0.000
0.000	0.858047	1297.48	692.289	0.000	0.000	0.855837	1287.09	705.328	0.000	0.000	0.000
0.046	0.852795	1285.48	709.618	-12.196	-0.080	0.046	0.850573	1275.21	722.978	-12.921	-0.082
0.106	0.845762	1270.40	732.607	-28.021	-0.169	0.106	0.843520	1259.95	746.789	-29.298	-0.175
0.212	0.833338	1242.91	776.783	-51.446	-0.311	0.212	0.831061	1232.38	792.278	-53.804	-0.320
0.299	0.822758	1219.79	816.879	-67.624	-0.403	0.299	0.820447	1209.15	833.660	-70.689	-0.415
0.402	0.809930	1190.71	870.844	-79.611	-0.458	0.402	0.807578	1179.95	889.382	-83.256	-0.472
0.503	0.798555	1165.53	921.825	-86.775	-0.505	0.503	0.796166	1154.73	941.967	-90.875	-0.521
0.600	0.784554	1134.25	990.740	-86.757	-0.492	0.600	0.782111	1123.15	1013.575	-90.604	-0.507
0.701	0.771175	1104.77	1062.437	-79.557	-0.447	0.701	0.768689	1093.71	1087.539	-83.422	-0.461
0.822	0.754617	1067.98	1161.842	-57.954	-0.336	0.822	0.752062	1056.78	1190.631	-60.888	-0.346
0.899	0.743666	1043.58	1234.726	-34.860	-0.213	0.899	0.741065	1032.26	1266.384	-36.688	-0.220
0.948	0.736543	1027.97	1284.816	-15.848	-0.090	0.948	0.733910	1016.58	1318.482	-16.770	-0.094
1.000	0.729112	1013.90	1334.183	0.000	0.000	1.000	0.726444	1002.41	1369.957	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.853622	1276.75	308.15K	0.000	0.000	0.000	0.851407	1266.54	310.65K	0.000	0.000
0.046	0.848347	1264.94	718.659	-13.623	-0.085	0.046	0.846119	1254.79	732.192	-14.354	-0.088
0.106	0.841274	1249.55	761.299	-30.633	-0.180	0.106	0.839024	1239.22	750.631	-31.974	-0.185
0.212	0.828779	1221.89	808.159	-56.255	-0.330	0.212	0.826493	1211.46	824.409	-58.768	-0.340
0.299	0.818132	1198.54	850.886	-73.866	-0.427	0.299	0.815815	1188.06	868.423	-77.257	-0.440
0.402	0.805218	1169.25	908.389	-87.079	-0.486	0.402	0.802853	1158.59	927.907	-91.025	-0.500
0.503	0.793770	1143.95	962.701	-95.110	-0.537	0.503	0.791367	1133.19	984.049	-99.463	-0.553
0.600	0.779660	1112.21	1036.862	-94.821	-0.522	0.600	0.777204	1101.37	1060.714	-99.321	-0.538
0.701	0.766192	1082.69	1113.407	-87.431	-0.476	0.701	0.763689	1071.77	1139.935	-91.736	-0.491
0.822	0.749497	1045.62	1220.344	-63.914	-0.357	0.822	0.746926	1034.57	1250.843	-67.243	-0.370
0.899	0.738451	1020.97	1299.129	-38.514	-0.227	0.899	0.735825	1009.77	1332.848	-40.538	-0.234
0.948	0.731264	1005.22	1353.330	-17.637	-0.097	0.948	0.728607	993.90	1389.381	-18.524	-0.101
1.000	0.723763	990.99	1406.906	0.000	0.000	1.000	0.721069	979.62	1445.133	0.000	0.000
0.000	0.849186	1256.29	746.135	0.000	0.000	0.000	0.846964	1246.12	760.353	0.000	0.000
0.046	0.843886	1244.61	764.979	-15.147	-0.091	0.046	0.841648	1234.49	779.640	-15.948	-0.093
0.106	0.836773	1228.98	791.230	-33.581	-0.192	0.106	0.834515	1218.74	806.759	-35.149	-0.197
0.212	0.824202	1201.05	841.093	-61.545	-0.350	0.212	0.821909	1190.79	858.037	-64.546	-0.361
0.299	0.813486	1177.49	886.616	-80.810	-0.453	0.299	0.811155	1166.93	905.329	-84.411	-0.467
0.402	0.800480	1147.95	947.990	-95.366	-0.516	0.402	0.798107	1137.45	968.443	-100.005	-0.532
0.503	0.788959	1122.50	1005.942	-104.354	-0.570	0.503	0.786547	1111.92	1028.320	-109.518	-0.588
0.600	0.774736	1090.47	1085.472	-104.143	-0.555	0.600	0.772257	1079.60	1110.996	-109.064	-0.571
0.701	0.761174	1060.84	1167.391	-96.479	-0.508	0.701	0.758651	1049.95	1195.696	-101.335	-0.524
0.822	0.744341	1023.44	1282.636	-70.806	-0.382	0.822	0.741744	1012.38	1315.403	-74.477	-0.394
0.899	0.733188	998.53	1367.925	-42.838	-0.242	0.899	0.730538	987.36	1404.126	-45.173	-0.249
0.948	0.725934	982.63	1426.668	-19.876	-0.105	0.948	0.723249	971.33	1465.475	-20.913	-0.109
1.000	0.718357	968.16	1485.133	0.000	0.000	1.000	0.715636	956.80	1526.390	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.844741	1236.06	318.15K	0.000	0.000	0.000	0.842518	1226.09	789.544	0.000	0.000
0.046	0.839413	1224.45	794.588	-16.754	-0.096	0.046	0.837173	1214.45	809.889	-17.549	-0.099
0.106	0.832261	1208.65	822.507	-36.855	-0.204	0.106	0.830003	1198.62	838.605	-38.648	-0.211
0.212	0.819612	1180.52	875.478	-67.520	-0.372	0.212	0.817315	1170.40	893.186	-70.830	-0.384
0.299	0.808784	1155.93	925.346	-87.274	-0.475	0.299	0.806474	1145.99	944.165	-92.076	-0.495
0.402	0.795730	1127.00	989.433	-104.783	-0.549	0.402	0.793356	1116.75	1010.695	-110.193	-0.569
0.503	0.784128	1101.38	1051.329	-114.823	-0.607	0.503	0.781711	1091.00	1074.742	-120.771	-0.628
0.600	0.769777	1068.91	1136.980	-114.413	-0.589	0.600	0.767333	1058.69	1162.729	-121.212	-0.615
0.701	0.756122	1039.17	1224.715	-106.474	-0.542	0.701	0.753581	1028.40	1254.717	-112.003	-0.560
0.822	0.739136	1001.40	1349.151	-78.295	-0.407	0.822	0.736516	990.46	1384.025	-82.551	-0.421
0.899	0.727875	976.23	1441.580	-47.465	-0.258	0.899	0.725199	965.11	1480.434	-50.044	-0.267
0.948	0.720551	960.13	1505.481	-22.016	-0.114	0.948	0.717839	948.99	1546.855	-23.512	-0.119
1.000	0.712897	945.54	1568.966	0.000	0.000	1.000	0.710141	934.24	1613.387	0.000	0.000
0.000	0.840306	1216.34	323.15K	0.000	0.000	0.000	0.842518	1226.09	789.544	0.000	0.000
0.046	0.834949	1204.70	825.244	-18.453	-0.102	0.102	0.837173	1214.45	809.889	-17.549	-0.099
0.106	0.827754	1188.80	854.833	-40.570	-0.217	0.217	0.830003	1198.62	838.605	-38.648	-0.211
0.212	0.815028	1160.49	911.055	-74.403	-0.397	0.397	0.806474	1145.99	944.165	-92.076	-0.495
0.299	0.804174	1136.30	963.084	-97.342	-0.515	0.515	0.793356	1116.75	1010.695	-110.193	-0.569
0.402	0.791012	1106.92	1031.774	-116.512	-0.592	0.592	0.781711	1091.00	1074.742	-120.771	-0.628
0.503	0.779302	1080.84	1098.427	-127.316	-0.651	0.651	0.767333	1058.69	1162.729	-121.212	-0.615
0.600	0.764898	1048.75	1188.646	-128.881	-0.642	0.642	0.753581	1028.40	1254.717	-112.003	-0.560
0.701	0.751042	1017.83	1285.243	-118.206	-0.579	0.579	0.736516	990.46	1384.025	-82.551	-0.421
0.822	0.733902	979.73	1419.545	-87.549	-0.436	0.436	0.725199	965.11	1480.434	-50.044	-0.267
0.899	0.722521	954.17	1520.190	-53.232	-0.276	0.276	0.717839	948.99	1546.855	-23.512	-0.119
0.948	0.715125	938.00	1589.324	-25.501	-0.124	0.124	0.710141	934.24	1613.387	0.000	0.000
1.000	0.707381	922.97	1659.478	0.000	0.000	0.000	0.700000	900.00	1666.667	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )	$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )
MTBE+isooctane											
0.000	0.695948	1124.31	288.15K	0.000	0.000	0.000	0.693910	1113.83	1161.606	0.000	0.000
0.049	0.697553	1121.76	1136.714	0.035	0.049	0.049	0.695495	1111.21	1164.431	2.149	0.035
0.091	0.698921	1119.48	1139.260	2.065	0.075	0.091	0.696847	1108.83	1167.166	4.304	0.075
0.197	0.702655	1113.86	1141.666	4.058	0.143	0.197	0.700534	1103.30	1172.691	8.371	0.145
0.296	0.706427	1108.70	1147.088	8.441	0.193	0.296	0.704261	1097.93	1177.923	12.242	0.195
0.394	0.710506	1103.74	1151.608	11.990	0.221	0.394	0.708292	1092.89	1182.047	15.012	0.222
0.507	0.715659	1098.54	1157.876	16.89	0.221	0.507	0.713386	1087.64	1184.964	16.379	0.222
0.603	0.720373	1094.92	1157.918	15.287	0.220	0.603	0.718048	1083.94	1185.321	15.411	0.221
0.700	0.725737	1090.87	1157.910	14.331	0.162	0.700	0.723357	1079.85	1185.552	14.312	0.162
0.790	0.731164	1087.76	1155.897	11.436	0.091	0.790	0.728726	1076.68	1183.757	11.279	0.090
0.898	0.738236	1084.61	1151.483	5.967	-0.010	0.898	0.735725	1073.34	1179.804	5.846	-0.012
0.951	0.742111	1083.37	1148.094	2.052	-0.081	0.951	0.739564	1071.99	1176.638	1.941	-0.084
1.000	0.744861	1082.11	1146.521	0.000	0.000	1.000	0.742259	1070.62	1175.368	0.000	0.000
0.000	0.691861	1103.30	1187.391	0.000	0.000	0.000	0.689809	1092.66	1214.230	0.000	0.000
0.049	0.693424	1100.63	1190.470	2.200	0.035879	0.049	0.691351	1089.97	1217.509	2.224	0.036
0.091	0.694760	1098.20	1193.445	4.419	0.076411	0.091	0.692668	1087.49	1220.743	4.550	0.078
0.197	0.698399	1092.59	1199.449	8.526	0.146906	0.197	0.696259	1081.81	1227.233	8.761	0.149
0.296	0.702081	1087.09	1205.263	12.566	0.197106	0.296	0.699893	1076.17	1233.692	13.089	0.200
0.394	0.706064	1082.04	1209.677	15.219	0.225176	0.394	0.703829	1071.08	1238.480	15.763	0.228
0.507	0.711097	1076.66	1213.149	16.672	0.225614	0.507	0.708799	1065.58	1242.524	17.382	0.229
0.603	0.715704	1072.87	1213.870	15.670	0.224712	0.603	0.713354	1061.73	1243.560	16.347	0.228
0.700	0.720957	1068.68	1214.494	14.562	0.164439	0.700	0.718545	1057.55	1244.355	15.063	0.168
0.790	0.726269	1065.47	1212.886	11.343	0.091936	0.790	0.7238	1054.18	1243.231	12.004	0.094
0.898	0.733196	1062	1209.291	5.8201	-0.01143	0.898	0.730656	1050.55	1240.091	6.548	-0.011
0.951	0.736997	1060.56	1206.324	1.891	-0.08466	0.951	0.734419	1049.03	1237.315	2.618	-0.085
1.000	0.739654	1059.10	1205.306	0.000	0.000	1.000	0.737036	1047.83	1235.747	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.687749	1082.20	298.15K	0.000	0.000	0.000	0.685687	1071.72	1269.730	0.000	0.000
0.049	0.689271	1079.41	1245.194	2.415	0.037	0.049	0.687187	1068.90	1273.652	2.450	0.038
0.091	0.690571	1076.87	1248.720	4.862	0.078	0.091	0.688468	1066.33	1277.418	4.950	0.080
0.197	0.694113	1071.16	1255.628	9.060	0.151	0.197	0.691962	1060.55	1284.859	9.212	0.153
0.296	0.697700	1065.45	1262.598	13.496	0.203	0.296	0.695502	1054.73	1292.466	13.847	0.205
0.394	0.701586	1060.20	1268.071	16.453	0.231	0.394	0.699338	1049.40	1298.467	16.897	0.234
0.507	0.706495	1054.67	1272.500	17.998	0.232	0.507	0.704182	1043.75	1303.533	18.582	0.236
0.603	0.710995	1050.73	1273.946	16.981	0.231	0.603	0.708630	1039.69	1305.488	17.647	0.234
0.700	0.716128	1046.37	1275.378	15.940	0.170	0.700	0.713701	1035.23	1307.405	16.664	0.173
0.790	0.721323	1042.91	1274.608	12.868	0.096	0.790	0.718837	1031.66	1307.063	13.623	0.098
0.898	0.728107	1039.23	1271.691	7.197	-0.011	0.898	0.725547	1027.87	1304.542	7.872	-0.011
0.951	0.731831	1037.63	1269.124	3.257	-0.086	0.951	0.729232	1026.19	1302.203	3.923	-0.087
1.000	0.734406	1036.63	1267.116	0.000	0.000	1.000	0.731766	1025.38	1299.745	0.000	0.000
0.000	0.683618	1061.30	1298.704	0.000	0.000	0.000	0.681542	1050.89	1328.596	0.000	0
0.049	0.685097	1058.43	1302.938	2.511	0.038	0.049	0.683001	1048.06	1332.927	2.341	0.038
0.091	0.686359	1055.84	1306.930	5.023	0.081	0.091	0.684244	1045.38	1337.336	5.040	0.081
0.197	0.689806	1050.01	1314.880	9.254	0.155	0.197	0.687643	1039.47	1345.901	9.307	0.156
0.296	0.693296	1044.04	1323.266	14.164	0.208	0.296	0.691083	1033.38	1355.032	14.422	0.210
0.394	0.697081	1038.65	1329.775	17.222	0.237	0.394	0.694818	1028.04	1361.786	17.188	0.239
0.507	0.701866	1032.83	1335.636	19.127	0.239	0.507	0.699540	1021.92	1368.843	19.674	0.241
0.603	0.706257	1028.69	1338.037	18.148	0.236	0.603	0.703873	1017.71	1371.695	18.621	0.239
0.700	0.711266	1024.11	1340.524	17.243	0.175	0.700	0.708820	1013.00	1374.818	17.824	0.177
0.790	0.716339	1020.42	1340.675	14.235	0.100	0.790	0.71383	1009.2	1375.469	14.826	0.101
0.898	0.722977	1016.51	1338.604	8.386	-0.011	0.898	0.720394	1005.18	1373.859	8.8504	-0.011
0.951	0.726622	1014.80	1336.382	4.280	-0.088	0.951	0.723998	1003.43	1371.793	4.607	-0.090
1.000	0.729112	1014.04	1333.815	0.000	0.000	1.000	0.726444	1002.70	1369.165	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )	$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )
0.000	0.679459	1040.53	308.15K	0.000	0.000	0.000	0.677373	1030.22	1390.952	0.000	0.000
0.049	0.680900	1037.69	1363.338	2.273	0.038	0.049	0.678790	1027.33	1395.869	2.314	0.039
0.091	0.682124	1034.98	1368.588	5.001	0.081	0.091	0.679994	1024.60	1400.833	5.040	0.083
0.197	0.685470	1029.03	1377.703	9.183	0.158	0.197	0.683293	1018.49	1410.846	9.433	0.159
0.296	0.688864	1022.78	1387.721	14.590	0.212	0.296	0.686637	1012.21	1421.450	14.784	0.214
0.394	0.692544	1017.58	1394.490	16.781	0.242	0.394	0.690270	1006.85	1429.063	17.182	0.244
0.507	0.697225	1011.05	1403.078	20.121	0.239	0.507	0.694875	1000.23	1438.446	20.587	0.243
0.603	0.701481	1006.79	1406.392	18.952	0.241	0.603	0.699077	995.90	1442.260	19.292	0.244
0.700	0.706365	1001.98	1410.109	18.169	0.179	0.700	0.703915	991.12	1446.196	18.102	0.178
0.790	0.711131	998.04	1411.384	15.255	0.103	0.790	0.708777	986.9	1448.585	15.718	0.105
0.898	0.717892	993.91	1410.267	9.125	-0.012	0.898	0.715208	982.76	1447.680	9.104	-0.015
0.951	0.721377	992.13	1408.317	4.677	-0.093	0.951	0.718741	981.15	1445.296	3.872	-0.097
1.000	0.723763	991.34	1405.913	0.000	0.000	1.000	0.721069	980.00	1444.013	0.000	0.000
0.000	0.675278	1019.94	1423.535	0.000	0.000	0.000	0.673177	1009.71	1457.060	0.000	0.000
0.049	0.676674	1017.02	1428.767	2.281	0.039	0.049	0.674551	1006.75	1462.655	2.274	0.039
0.091	0.677857	1014.35	1433.792	4.770	0.084	0.091	0.675716	1003.97	1468.231	4.995	0.084
0.197	0.681108	1007.98	1445.041	9.647	0.160	0.197	0.678915	997.54	1480.212	9.805	0.162
0.296	0.684416	1001.85	1455.709	14.359	0.212	0.296	0.682172	991.38	1491.509	14.399	0.215
0.394	0.687984	996.15	1464.779	17.516	0.245	0.394	0.685682	985.48	1501.695	17.929	0.248
0.507	0.692513	989.48	1474.885	20.843	0.247	0.507	0.690141	978.73	1512.643	21.250	0.252
0.603	0.696659	984.99	1479.504	19.672	0.247	0.603	0.694229	974.09	1518.095	20.185	0.251
0.700	0.701432	980.08	1484.196	18.552	0.180	0.700	0.698938	969.06	1523.562	19.109	0.184
0.790	0.706232	975.76	1487.190	16.135	0.107	0.790	0.703665	964.56	1527.480	16.938	0.111
0.898	0.712585	971.49	1486.917	9.387	-0.015	0.898	0.709948	960.23	1527.647	9.819	-0.015
0.951	0.716075	969.68	1485.199	4.442	-0.098	0.951	0.713392	958.31	1526.370	4.909	-0.098
1.000	0.718357	968.63	1483.692	0.000	0.000	1.000	0.715636	957.31	1524.764	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.671069	999.53	318.15K	0.000	0.000	0.000	0.668954	989.37	320.65K	0.000	0.000
0.049	0.672418	996.53	1497.545	2.266	0.040	0.049	0.670282	986.33	1527.166	2.242	0.040
0.091	0.673564	993.65	1503.676	5.202	0.086	0.091	0.671436	983.34	1533.550	5.371	0.079
0.197	0.676709	987.14	1516.493	9.993	0.165	0.197	0.674493	976.73	1554.080	10.271	0.167
0.296	0.679911	980.84	1528.803	14.801	0.218	0.296	0.677642	970.30	1567.428	15.260	0.222
0.394	0.683366	974.83	1539.887	18.435	0.253	0.394	0.681043	964.20	1579.397	18.929	0.256
0.507	0.687763	968.07	1551.485	21.496	0.255	0.507	0.685370	957.34	1591.998	22.019	0.259
0.603	0.691788	963.20	1558.095	20.811	0.254	0.603	0.689334	952.36	1599.440	21.334	0.258
0.700	0.696427	958.04	1564.434	19.827	0.187	0.700	0.693905	947.08	1606.670	20.406	0.191
0.790	0.701097	953.55	1568.682	17.259	0.113	0.790	0.698504	942.46	1611.778	17.920	0.116
0.898	0.707292	949.03	1569.789	10.212	-0.014	0.898	0.704622	937.81	1613.668	10.725	-0.013
0.951	0.711093	947.02	1568.916	5.273	-0.098	0.951	0.707978	935.72	1613.201	5.728	-0.098
1.000	0.712897	946.03	1567.341	0.000	0.000	1.000	0.710141	934.76	1611.592	0.000	0.000
0.000	0.6666832	979.25	1563.855	0.000	0.000						
0.049	0.6668138	976.18	1570.630	2.171	0.041						
0.091	0.669267	973.04	1578.117	5.700	0.081						
0.197	0.672267	966.34	1592.936	10.577	0.171						
0.296	0.675361	959.80	1607.321	15.670	0.227						
0.394	0.678707	953.63	1620.160	19.281	0.262						
0.507	0.682969	946.69	1633.742	22.289	0.264						
0.603	0.686867	941.57	1642.185	21.696	0.264						
0.700	0.691375	936.24	1650.106	20.549	0.195						
0.790	0.695909	931.51	1656.046	18.046	0.119						
0.898	0.701938	926.65	1659.089	10.988	-0.010						
0.951	0.705250	924.50	1658.987	5.850	-0.097						
1.000	0.707381	923.46	1657.717	0.000	0.000						

**Table 2** continued

$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )	$x_1$	$\rho$ (g · cm <sup>-3</sup> )	$u$ (m · s <sup>-1</sup> )	$\kappa_S$ (TPa <sup>-1</sup> )	$\delta\kappa_S$ (TPa <sup>-1</sup> )	$V^E$ (cm <sup>3</sup> · mol <sup>-1</sup> )
301.65 K											
0.000	0.777762	1108.98	1045.456	0.000	0.000	0.000	0.775212	1099.02	1067.993	0.000	0.000
0.049	0.775452	1105.41	1055.354	-2.554	-0.062	0.049	0.772916	1094.69	1079.656	-1.377	-0.066
0.100	0.772914	1100.67	1067.959	-2.934	-0.104	0.100	0.770395	1090.25	1092.029	-2.601	-0.110
0.215	0.767025	1089.35	1098.641	-1.351	-0.140	0.215	0.764529	1079.09	1123.287	-1.817	-0.152
0.314	0.761986	1079.69	1125.783	0.500	-0.147	0.314	0.759479	1069.65	1150.803	-0.787	-0.159
0.400	0.757940	1072.04	1148.003	0.818	-0.170	0.400	0.755424	1061.93	1173.863	-0.663	-0.183
0.498	0.753459	1063.59	1173.254	1.89	-0.185	0.498	0.750928	1053.12	1200.732	0.152	-0.198
0.597	0.749177	1055.55	1198.003	0.706	-0.208	0.597	0.746615	1045.00	1226.509	-0.495	-0.218
0.707	0.744495	1047.57	1223.974	-1.086	-0.206	0.707	0.741905	1036.67	1254.211	-1.866	-0.213
0.799	0.740646	1040.83	1246.320	-2.141	-0.192	0.799	0.738033	1029.86	1277.520	-3.064	-0.197
0.900	0.736522	1033.08	1272.174	-2.081	-0.167	0.900	0.733889	1021.91	1304.801	-2.795	-0.171
0.951	0.734553	1028.81	1286.194	-0.923	-0.158	0.951	0.731913	1017.59	1319.456	-1.610	-0.161
1.000	0.731766	1025.42	1299.643	0.000	0.000	1.000	0.729112	1013.90	1334.183	0.000	0.000
MTBE + <i>tert</i> -butyl alcohol											
0.000	0.772623	1088.33	1092.726	0.000	0.000	0.000	0.770015	1077.71	1118.142	0.000	0.000
0.049	0.770344	1083.98	1104.772	-1.535	-0.069	0.049	0.767747	1073.25	1130.785	-1.503	-0.071
0.100	0.767841	1079.68	1117.220	-3.249	-0.117	0.100	0.765265	1069.10	1143.277	-3.762	-0.123
0.215	0.762002	1068.69	1149.054	-3.151	-0.165	0.215	0.759448	1058.21	1175.867	-4.229	-0.176
0.314	0.756946	1059.44	1177.016	-2.774	-0.173	0.314	0.754398	1049.11	1204.363	-4.465	-0.186
0.400	0.752889	1051.72	1200.795	-2.883	-0.198	0.400	0.750325	1041.22	1229.322	-4.388	-0.210
0.498	0.748373	1042.61	1229.244	-1.568	-0.211	0.498	0.745794	1032.03	1258.915	-3.057	-0.223
0.597	0.744023	1034.29	1256.403	-1.930	-0.228	0.597	0.741414	1023.49	1287.573	-3.064	-0.237
0.707	0.739304	1025.94	1285.088	-3.523	-0.223	0.707	0.736686	1015.17	1317.165	-5.012	-0.232
0.799	0.735393	1018.70	1310.352	-3.784	-0.201	0.799	0.732737	1007.62	1344.183	-4.579	-0.205
0.900	0.731231	1010.60	1339.019	-3.248	-0.173	0.900	0.728559	999.39	1374.249	-3.815	-0.175
0.951	0.729253	1006.29	1354.177	-2.119	-0.163	0.951	0.726577	994.94	1390.351	-2.325	-0.165
1.000	0.726444	1002.41	1369.957	0.000	0.000	1.000	0.723763	990.99	1406.906	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.767391	1067.22	310.65 K	0.000	0.000	0.000	0.764739	1056.73	313.15 K	0.000	0.000
0.049	0.765130	1062.61	1144.130	-1.387	-0.073	0.049	0.762492	1052.05	1171.005	-1.466	-0.076
0.100	0.762685	1058.87	1157.489	-4.834	-0.131	0.100	0.760064	1048.39	1184.928	-5.413	-0.137
0.215	0.756880	1047.90	1169.417	-5.522	-0.187	0.215	0.754270	1037.39	1231.939	-6.462	-0.197
0.314	0.751817	1038.63	1233.009	-5.652	-0.198	0.314	0.749212	1028.16	1262.623	-7.033	-0.209
0.400	0.747731	1030.64	1259.043	-5.553	-0.221	0.400	0.745126	1020.25	1289.309	-7.414	-0.234
0.498	0.743186	1021.35	1289.892	-4.165	-0.233	0.498	0.740567	1010.91	1321.328	-6.141	-0.245
0.597	0.738784	1012.78	1319.630	-4.307	-0.245	0.597	0.736130	1002.02	1352.984	-5.668	-0.253
0.707	0.734036	1004.28	1350.744	-6.069	-0.238	0.707	0.731360	993.34	1385.712	-7.249	-0.244
0.799	0.730062	996.52	1379.330	-5.195	-0.208	0.799	0.727372	985.44	1415.739	-6.144	-0.212
0.900	0.725873	988.12	1410.977	-4.091	-0.176	0.900	0.723168	976.81	1449.241	-4.517	-0.178
0.951	0.723884	983.57	1427.975	-2.326	-0.166	0.951	0.721205	972.48	1466.155	-3.498	-0.172
1.000	0.721069	979.62	1445.133	0.000	0.000	1.000	0.718357	968.16	1299.643	0.000	0.000
0.000	0.762054	1046.12	1199.089	0.000	0.000	0.000	0.759355	1035.66	318.15 K	0.000	0.000
0.049	0.759831	1041.53	1213.220	-1.903	-0.080	0.049	0.757138	1031.00	1227.781	0.000	0.000
0.100	0.757407	1037.81	1225.843	-5.999	-0.143	0.100	0.754279	1027.28	1242.532	-1.963	-0.082
0.215	0.751633	1026.85	1261.770	-7.541	-0.206	0.215	0.748972	1016.34	1255.542	-6.381	-0.147
0.314	0.746577	1017.66	1293.362	-8.516	-0.220	0.314	0.743917	1007.14	1292.577	-8.404	-0.215
0.400	0.742483	1009.68	1321.131	-8.948	-0.245	0.400	0.739814	999.06	1325.244	-9.686	-0.230
0.498	0.737910	1000.24	1354.529	-7.585	-0.255	0.498	0.735227	989.54	1354.236	-10.092	-0.254
0.597	0.733459	991.47	1386.963	-7.642	-0.261	0.597	0.730762	980.67	1422.913	-8.678	-0.268
0.707	0.728662	982.37	1422.079	-8.274	-0.248	0.707	0.725943	971.38	1459.887	-8.968	-0.252
0.799	0.724660	974.33	1453.629	-6.857	-0.214	0.799	0.721933	963.24	1492.912	-7.355	-0.217
0.900	0.720449	965.56	1488.806	-4.892	-0.180	0.900	0.717738	954.55	1529.103	-5.785	-0.185
0.951	0.718495	961.27	1506.210	-4.051	-0.175	0.951	0.715752	949.91	1548.362	-3.791	-0.176
1.000	0.715636	956.80	1526.390	0.000	0.000	1.000	0.712897	945.54	1568.966	0.000	0.000

**Table 2** continued

$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )	$x_1$	$\rho$ (g · cm $^{-3}$ )	$u$ (m · s $^{-1}$ )	$\kappa_S$ (TPa $^{-1}$ )	$\delta\kappa_S$ (TPa $^{-1}$ )	$V^E$ (cm $^3$ · mol $^{-1}$ )
0.000	0.756633	1025.17	323.15K	0.000	0.000	0.000	0.753891	1014.76	323.15K	0.000	0.000
0.049	0.754421	1020.47	1257.543	0.000	-0.084	0.049	0.751680	1009.99	1288.145	0.000	-0.085
0.100	0.752024	1016.75	1272.875	-2.101	-0.151	0.100	0.749295	1006.31	1304.166	-2.170	-0.155
0.215	0.746283	1005.85	1286.293	-6.860	-0.223	0.215	0.743567	995.37	1317.903	-7.401	-0.229
0.314	0.741230	996.62	1324.433	-9.456	-0.239	0.314	0.738520	986.19	1357.409	-10.405	-0.246
0.400	0.737119	988.47	1358.275	-11.021	-0.263	0.400	0.734400	977.86	1392.248	-12.514	-0.270
0.498	0.732517	978.82	1388.467	-11.490	-0.270	0.498	0.729786	968.08	1424.013	-12.745	-0.276
0.597	0.728042	969.80	1424.875	-9.911	-0.274	0.597	0.725316	958.97	1462.116	-10.985	-0.281
0.707	0.723201	960.40	1460.425	-9.685	-0.255	0.707	0.720436	949.42	1499.211	-10.753	-0.256
0.799	0.719199	952.31	1519.121	-9.854	-0.222	0.799	0.716426	941.22	1539.883	-10.638	-0.221
0.900	0.714978	943.30	1533.184	-8.552	-0.186	0.900	0.712195	931.99	1575.601	-9.107	-0.183
0.951	0.712991	938.58	1571.838	-6.007	-0.176	0.951	0.710215	927.25	1616.511	-5.878	-0.175
1.000	0.710141	934.24	1592.111	-3.740	0.000	1.000	0.707381	922.97	1637.633	-3.547	0.000

No previous data have been found over the entire range of temperatures studied for these binary mixtures. Only a few collections of data related to excess volume were found at a few temperatures [17–20]. As far as we know, no previous comprehensive study has been carried out, involving sound speeds. Comparisons of the fitted excess volumes for the binary mixtures of MTBE+ (benzene, toluene, ethylbenzene, isoctane, and TBA) with open literature data have been plotted in Fig. 3.

### 3.2 Collision Factor and Free Length Theories

Experimental data for the deviations of the isentropic compressibility of the mixtures were compared with values from different theories. The collision factor theory (CFT) [5, 6, 21] and free length theory (FLT) [4, 21] for isentropic compressibilities are expressed, respectively, as follows:

$$\kappa_S = \left( \frac{1}{\rho^3} \right) \left( \frac{M}{u_\infty \sum_i^N x_i S_s \sum_i^N x_i B_s} \right)^2 \quad (2)$$

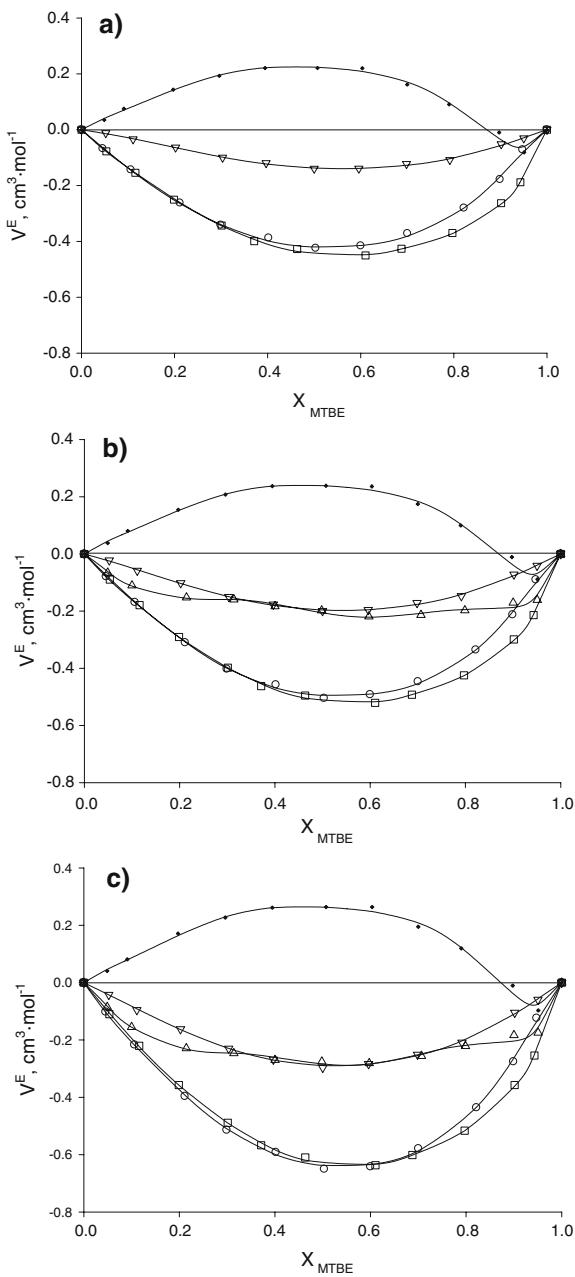
$$\kappa_S = \left( \frac{L_f^2}{K^2} \right) \quad (3)$$

The collision factor theory (CFT) is dependent on the collision factors among molecules in a pure solvent or mixture as a function of temperature. The pertinent relations in these calculations and their theoretical basis were described in the literature cited above. The collision factors ( $S$ ) and the characteristic molecular volumes ( $B$ ) of the pure solvents used in the CFT calculations were estimated by using the experimental sound speeds from this paper, and the corresponding molar volumes. These values could also be evaluated by means of the group contribution method proposed by Schaffs [22] when no experimental data are available. The root-mean-square deviations presented were computed using the following equation, where  $z$  is the value of the derived magnitude, and  $n_{DAT}$  is the number of experimental data:

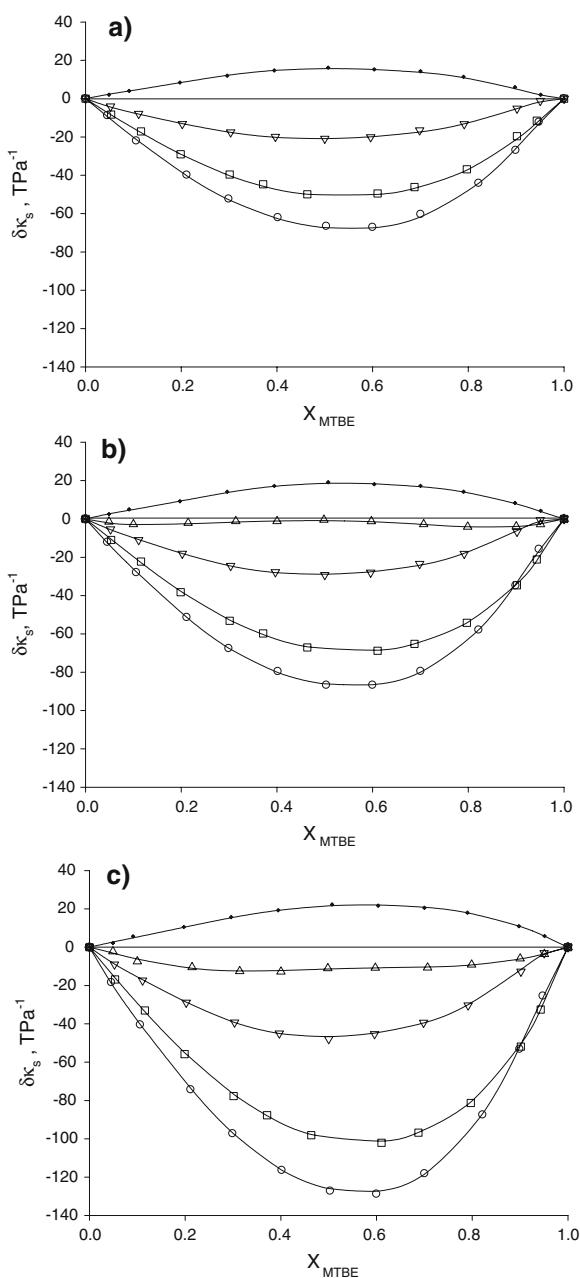
$$\sigma = \left( \frac{\sum_{i=1}^{n_{DAT}} (z_{exp} - z_{pred})^2}{n_{DAT}} \right)^{1/2} \quad (4)$$

The free length theory is used to estimate the isentropic compressibility of a mixture depending on the free displacement of molecules as a function of temperature. In the last few years different authors have compared the relative merits of existing theories with the free length theory, and found that the use of the FLT gives smaller deviations

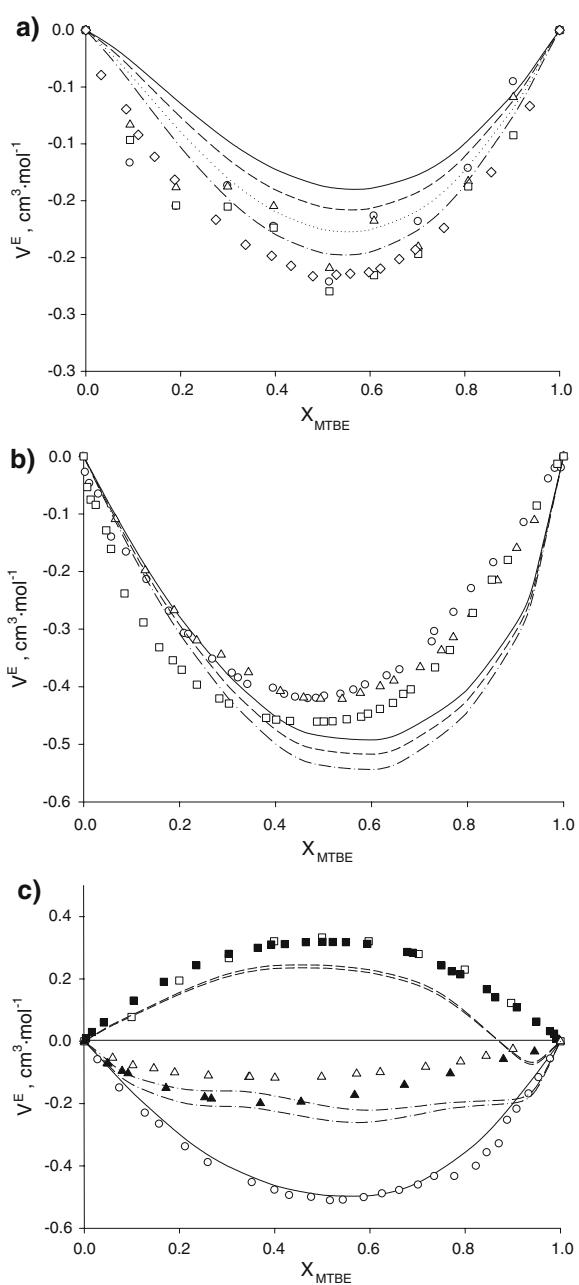
**Fig. 1** Excess molar volumes of mixtures of MTBE + (▽, benzene; □, toluene; ○, ethylbenzene; ●, isooctane; △, *tert*-butyl alcohol) at (a) 288.15 K, (b) 298.15 K, and (c) 323.15 K. Solid lines represent Redlich–Kister fitted curves



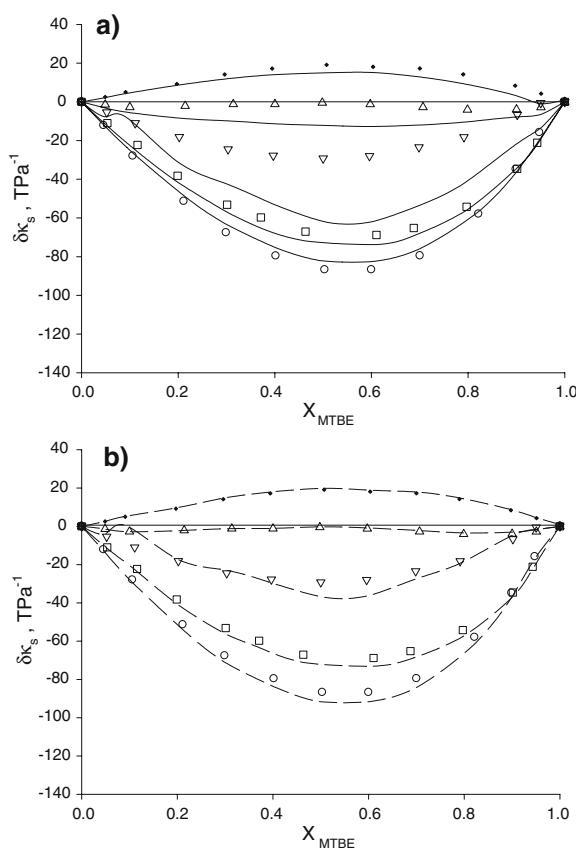
**Fig. 2** Deviations of isentropic compressibility of mixtures of MTBE+ $(\nabla$ , benzene;  $\square$ , toluene;  $\circ$ , ethylbenzene;  $\bullet$ , isooctane;  $\triangle$ , *tert*-butyl alcohol at (a) 288.15 K, (b) 298.15 K, and (c) 323.15 K. Solid lines represent Redlich–Kister fitted curves



**Fig. 3** Comparisons of the fitted excess volume of mixtures with open literature results of (a) MTBE + benzene (at 288.15 ○ [17], experimental data (—); at 293.15 △ [17], experimental data (—); at 298.15 □ [17], experimental data (· · ·); at 303.15 ◇ [17], experimental data (---)); (b) MTBE + toluene (at 298.15 ○ [19], experimental data (—); at 303.15 △ [18], experimental data (—); at 308.15 □ [19], experimental data (· · ·)); and (c) MTBE + ethylbenzene (at 303.15 ○ [18], experimental data (—)), MTBE + isooctane (at 298.15 □ [10] and at 308.15 ● [19], experimental data (—)), MTBE + TBA (at 303.15 △ [12] and at 313.15 ● [20], experimental data (---))



**Fig. 4** Comparisons of the experimental deviations of isentropic compressibility ( $\text{TPa}^{-1}$ ) and those fitted by (a) CFT (continuous line) and (b) FLT (dashed line) of mixtures of MTBE+( $\nabla$ , benzene;  $\square$ , toluene;  $\circ$ , ethylbenzene;  $\bullet$ , isoctane;  $\triangle$ , *tert*-butyl alcohol) at 303.15 K



**Table 3** Root-mean-square deviations for estimated deviations of isentropic compressibilities from experimental data for the mixtures from 288.15 to 323.15 K

Mixture	CFT (Eq. 2)			FLT (Eq. 3)		
	288.15 K	303.15 K	323.15 K	288.15 K	303.15 K	323.15 K
MTBE + ethylbenzene	2.857	3.302	4.835	0.551	3.373	13.332
MTBE + isoctane	2.100	3.541	5.038	0.290	0.514	2.020
MTBE + benzene	17.498	21.633	10.286	0.806	2.338	6.583
MTBE + toluene	5.234	3.561	4.034	0.124	3.036	11.259
MTBE + TBA	--	8.301	6.806	--	0.329	1.670

of computed isentropic compressibilities when compared with experimental values [8]. The deviations for each theory for the studied mixtures are reported in Table 3. In Fig. 4 the uncertainty of the models can be estimated for the binaries mixtures at 303.15 K, using comparisons.

#### 4 Discussion and Conclusions

The phase equilibria and excess properties for systems containing ethers, alcohols, and hydrocarbons have been the subject of numerous studies in the past few years. Nevertheless, more data are required to develop solution models and to design process separation units. For this aim, we present in this paper the temperature dependence of the density and sound speeds of binary mixtures of MTBE + (benzene, toluene, ethylbenzene, isoctane, and TBA) over the range from 288.15 to 323.15 K and at atmospheric pressure, as a function of composition. For each system of this study, a slight dependence on temperature is observed over the studied range. The contractive behavior of the mixtures of MTBE + (benzene, toluene, ethylbenzene, and TBA) increases at higher temperatures. Only the binary system MTBE + isoctane shows expansive behavior with an increase in temperature. This mixture show a small gap in the negative trend at high MTBE compositions due to the capability of the oxygen molecular group in the ether molecule to create dipole interactions among MTBE molecules. This negative gap was confirmed at any temperature and by repeated measurements. This behavior is in conflict with open literature results [10, 19]. It is worthwhile to point out a similar behavior for the aryl compounds, as expected, although a slight difference for MTBE + (benzene and toluene) between our experimental data and available literature results was observed. TBA was studied from 301.65 K due to its high melting point, thus, there was no possibility to calculate excess properties at lower temperatures. The case for a TBA is a little different; it is a product of degradation of MTBE and a persistent pollutant due to its strong interaction with pseudo-polar media. Interactions between a polar component such as an alcohol, and an ether are suggested to occur via complex formation between the two species between the unshared electron pairs on the oxygen atom of an ether molecule and a hydroxyl group of an alcohol. The excess molar volume is usually reported as negative and as a function of steric hindrance. The excess molar volumes for mixtures of TBA with globular ethers such as MTBE are much lower than for similar *n*-ethers with shorter alcohols.

In terms of isentropic compressibilities, a similar trend was observed; positive deviations were obtained only for MTBE + isoctane (Fig. 2). This trend would seem to indicate: (a) a more organized packing effect in equimolar compositions of MTBE + (benzene, toluene, ethylbenzene, and TBA), (b) breakdown of ether–ether interactions for the mixture MTBE + isoctane when the MTBE composition decreases, and (c) positive effect for this binary mixture due to the stronger specific interactions of aliphatic ends by steric hindrance interactions.

In terms of isentropic compressibility and considering the deviations with computed data, we arrive at the conclusion that the application of the free length theory to predict experimental data has been successful for all the studied mixtures, showing this procedure as a reliable tool for calculation of the isentropic compressibility for these kinds of systems.

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