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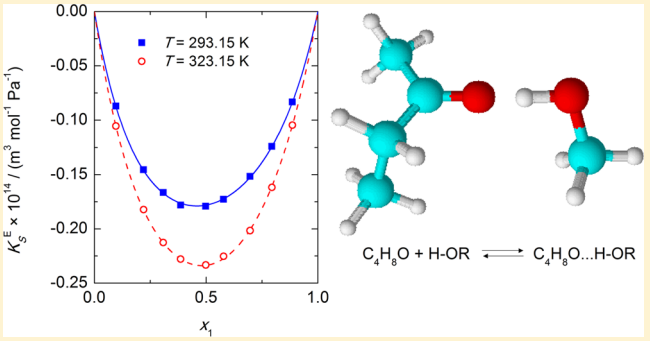
Speed of Sound, Density, and Related Thermodynamic Excess Properties of Binary Mixtures of Butan-2-one with C1−C4 *n*-Alkanols and Chloroform

Mikhail A. Varfolomeev,[†] Ksenia V. Zaitseva,[†] Ilnaz T. Rakipov,[†] Boris N. Solomonov,[†] and Wojciech Marczak*[,†,‡]

[†]Department of Physical Chemistry, Kazan Federal University, Kremlevskaya str. 18, 420008 Kazan, Russian Federation

[‡]Institute of Occupational Medicine and Environmental Health, Kościelna 13, 41-200 Sosnowiec, Poland

ABSTRACT: Densities and speeds of sound were measured for binary mixtures of butan-2-one with methanol, propan-1-ol, butan-1-ol, and chloroform at temperatures of 293.15−323.15 K and at atmospheric pressure, with the uncertainties of 0.05 kg·m^{-3} and 0.5 m·s^{-1}, respectively. The molar excesses of volume, isentropic compression, and thermal expansion were calculated for those systems from the measured speeds and densities and for the mixture of butan-2-one with ethanol from the data reported in the literature. The negative excess volumes for the mixtures with alcohols decrease with the elongation of the hydrocarbon chain, and they eventually become positive for propan-1-ol and butan-1-ol at higher temperatures. That probably reflects the vanishing difference in size of the molecules in the mixture. The excess volume of butan-2-one + chloroform is close to that of butan-2-one + methanol. The excess expansion of butan-2-one + chloroform is negative, and it is positive for butan-2-one + alcohols, while the excess compression isotherms are approximately mirror images of those of the excess expansion. That results probably from the counteracting effects of temperature and pressure on the aggregation due to hydrogen bonds.



INTRODUCTION

Butan-2-one is a popular industrial solvent manufactured by extraction from the mixtures containing carbonyls and alcohols obtained in the Fischer−Tropsch reaction.[1] It forms azeotropes with various alcohols that makes the purification process difficult. For that reason, detailed studies of the vapor−liquid equilibria have been undertaken in the last years.[2] The thermodynamic nonideal behavior of the mixtures of butan-2-one with alcohols is manifested also in the excesses of enthalpy and volume.[2−12] However, information about the compressibility of butan-2-one + alcohols is scarce. The compressibility and speed of sound for butan-2-one + methanol was reported by Abraham,[13] for butan-2-one + ethanol by Pereiro and Rodriguez,[7] for butan-2-one + propan-1-ol and butan-2-one + butan-1-ol by Reddy,[14] but the excess molar compressions were not calculated. Moreover, the speed of sound in methanol and its density measured by Abraham[13] were higher than those reported by other authors by ca. 7 m·s^{-1} and 2.5 kg·m^{-3}, both of which obviously affected the calculated compressibility.

In the present work, we report experimental densities and speeds of sound for binary mixtures of butan-2-one with methanol, propan-1-ol, butan-1-ol, and chloroform measured at different temperatures. The thermodynamic excesses of volume, thermal expansion, and isentropic compression were calculated for these systems from the experimental results, and for butan-2-one + ethanol from the data reported by Pereiro and Rodriguez.[7] The butan-2-one + chloroform system was chosen as a reference, where no hydrogen bonds occur in pure liquids.

This work was aimed mainly at collecting data necessary in the studies of hydrogen-bonded liquid systems. Both the isentropic compression, being the second-order pressure derivative of enthalpy, $K_S = -(\partial^2 H/\partial p^2)_S$, as well as the volume, $V = (\partial H/\partial p)_S$, are thermal characteristics of liquids important from the fundamental point of view and useful in the industrial applications.

EXPERIMENTAL SECTION

Chemicals. Butan-2-one, methanol, propan-1-ol, butan-1-ol, and chloroform were dried over molecular sieves of 4 Å and distilled using a rectifying column. The purity of the studied compounds was checked using an Agilent 7890B gas chromatograph with a flame ionization detector. Residual water content was determined by the Karl Fischer titration. In each binary system, butan-2-one from different production batches was used. In spite of the same purification procedure, slight differences in the density of the samples of butan-2-one and in the speed of sound were found. That probably resulted mainly from different

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Table 1. Characteristics of the Chemicals Used in the Experiment; Density (ρ) and Speed of Sound (u) at T = 298.15 K

							ρ/kg·m^{-3}		u/m·s^{-1}	
chemical name	source	initial mass fraction purity	purification method	final mass fraction purity	analysis method	mass fraction of water·100	measured	literature	measured	literature
butan-2-one	Aldrich	0.98	distillation	0.999	GC[a]	0.04	799.60	799.61[b]	1192.06	1192.2[c]
	Aldrich	0.98	distillation	0.999	GC		799.68	799.62[d]	1192.14	
	Aldrich	0.98	distillation	0.999	GC		799.74	799.68[e]	1191.97	
	Aldrich	0.98	distillation	0.999	GC		799.94	799.7[f]	1193.15	
								799.74[g]		
								799.891[h]		
								800.05[i]		
								800.1[c]		
methanol	Aldrich	0.98	distillation	0.999	GC	0.02	786.58	786.6[c]	1102.81	1102.1[c]
								787.727[j]		
propan-1-ol	Aldrich	0.98	distillation	0.999	GC	0.02	799.47	799.44[d]	1205.64	1204.85[k]
								799.46[k]		
butan-1-ol	Aldrich	0.98	distillation	0.999	GC	0.03	805.81	805.48[b]	1240.37	1240.25[l]
								805.81[l]		
								805.823[j]		
chloroform	Aldrich	0.98	distillation	0.999	GC	0.04	1478.16	1472.435[m]	983.68	983.58[m]
								1478.5[h]		
								1479.25[j]		

[a]Gas chromatography. [b]Martínez et al.[4]. [c]M. Iglesias et al.[12]. [d]Martínez et al.[2]. [e]Hsu-Chen Ku and Chein-Hsiun Tu[6]. [f]Pereiro and Rodríguez[7]. [g]Comelli and Francesconi[15]. [h]Faranda et al.[5]. [i]Clará et al.[16]. [j]DDBST[17]. [k]Marczak and Spurek[18]. [l]Zorębski et al.[19]. [m]Bhatia et al.[20].

concentrations of water. Commonly for organic liquids, even small contamination by water causes an evident increase of the density and speed of sound. Characteristics of the chemicals are reported in Table 1. The measured densities and speeds of sound agree well with those reported in the literature.

The solutions were prepared by weighing of the chemicals in bottles with airtight stoppers, using an analytical balance with an accuracy of $\pm 1 \cdot 10^{-4}$ g. The less volatile component of the mixture was injected into the bottle as the first one. Each mixture was used immediately after it was well mixed by shaking. Tightness of the seals was checked by weighting randomly chosen bottles twice: first, just after the filling with butan-2-one and next, after a break of 1 h. No mass change evidenced that the chemical neither evaporated, nor absorbed the air moisture.

Taking into account the balance accuracy and the sample size, the uncertainty in the mole fraction was estimated as $5 \cdot 10^{-5}$.

Apparatus. The density and sound velocity meter Anton Paar DSA 5000 was used in the measurements. The apparatus was calibrated with water and dry air following the instructions and requirements of the manufacturer. Calibrations were performed at a temperature of 293.15 K. The temperature was controlled by built-in Peltier thermostat to within ±0.002 K. The measurement resolution was $1 \cdot 10^{-3}$ kg m^{-3} for the density and $1 \cdot 10^{-2}$ m s^{-1} for the speed of sound, while the uncertainties were estimated for $5 \cdot 10^{-2}$ kg m^{-3} and $5 \cdot 10^{-1}$ m s^{-1}, respectively. In the evaluation of the uncertainties, the principles of the measurement techniques as well as the attainable quality of the standard water were taken into account.

RESULTS

The speed of sound (u) and density (ρ) were measured for pure liquids and for binary mixtures of butan-2-one with methanol, propan-1-ol, and butan-1-ol at temperatures from 293.15 to 323.15 K in 5 K intervals. For the mixture of butan-2-one with chloroform, the upper temperature of the measurements was 308.15 K because of rather high vapor pressure of chloroform at higher temperatures. Comparisons of the densities and speeds measured in this study and reported in literature sources are given in Figures 1−6.

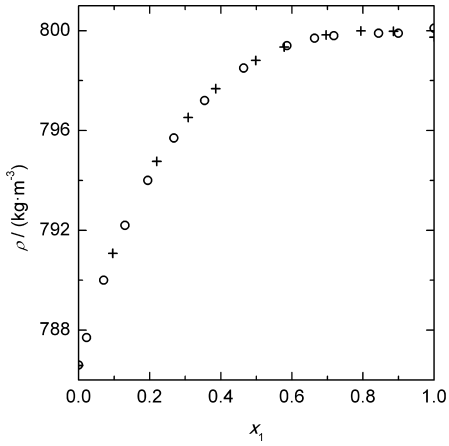

Figure 1. Density of binary system butan-2-one (1) + methanol (2) at T = 298.15 K: + − this work, ○ − Iglesias et al.[12]

From the experimental densities and speeds, the isentropic compressibilities were calculated using the Laplace formula:

$$\kappa_S = \rho^{-1} u^{-2} \quad (1)$$

The results are reported in Tables 2−5.

The dependencies of specific volume ($\nu \equiv \rho^{-1}$) on temperature (T) were approximated by the following equation:

$$\ln[\nu/(\mathrm{cm}^3 \cdot \mathrm{g}^{-1})] = \ln \nu_{25} + \sum_{i=1}^{3} a_i \vartheta^i \quad (2)$$

where $\vartheta = T/\mathrm{K} - 298.15$, the value of ν_{25} is equal to the specific volume at T = 298.15 K given in cm^3·g^{-1}, and a_i are the empirical coefficients. The ln ν_{25} and statistically significant a_i coefficients were obtained by the least-squares fit of eq 2. The fit applied the stepwise backward rejection procedure based on the results of the F-testing. For the system butan-2-one + chloroform,

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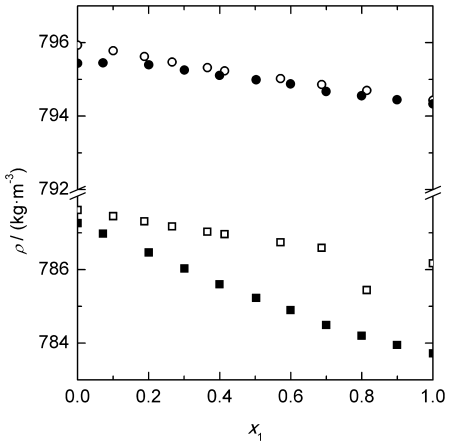

Figure 2. Density of binary system butan-2-one (1) + popan-1-ol (2). This work: ● − T = 303.15 K, ■ − T = 313.15 K; Reddy and Naidu:[14] ○ − T = 303.15 K, □ − T = 313.15 K.

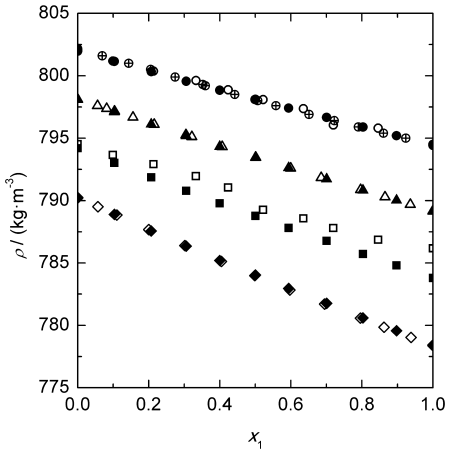

Figure 3. Density of binary system butan-2-one (1) + butan-1-ol (2). This work: ● − T = 303.15 K, ▲ − T = 308.15 K, ■ − T = 313.15 K, ◆ − T = 318.15 K; Reddy and Naidu:[14] ○ − T = 303.15 K, □ − T = 313.15 K; Martínez et al.:[4] Δ − T = 308.15 K, ◇ − T = 318.15 K; Clará, Gómez Marigliano and Sólimo:[8] ⊕ − T = 303.15 K.

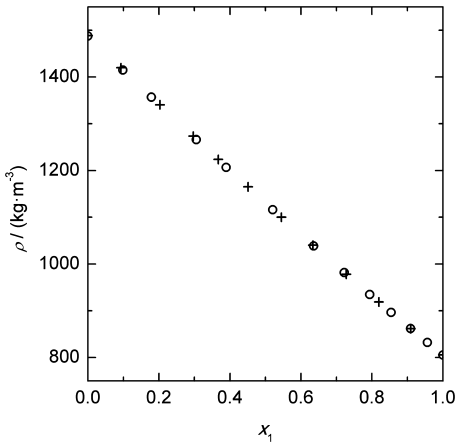

Figure 4. Density of binary system butan-2-one (1) + chloroform (2) at T = 293.15 K: + − this work, ○ − Clará, Gómez Marigliano and Sólimo.[16]

the second-order polynomials were used for the interpolation by default rather than the third-order eq 2 because of rather narrow temperature range of the measurements. Any density calculated

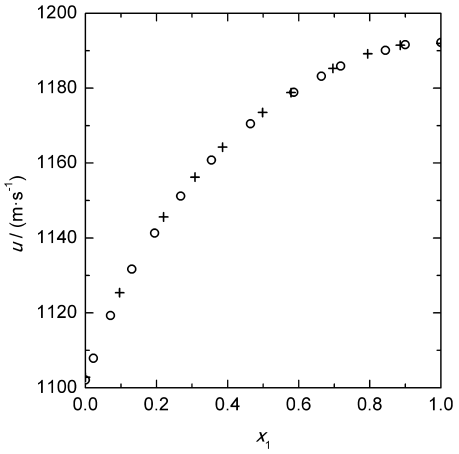

Figure 5. Speed of sound in binary systems butan-2-one (1) + methanol (2) at T = 298.15 K: + − this work, ○ − Iglesias et al.[12]

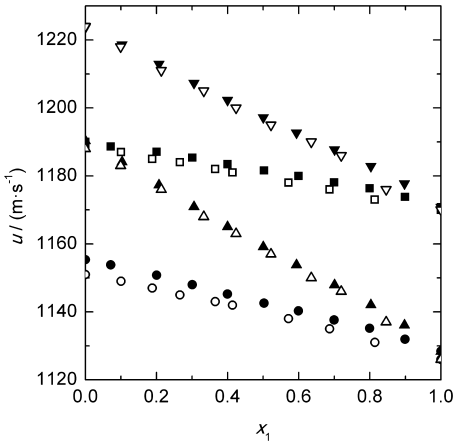

Figure 6. Speed of sound in binary systems butan-2-one (1) + alcohol (2). This work, propan-1-ol: ■ − T = 303.15 K, ● − T = 313.15 K; butan-1-ol: ▼ − T = 308.15 K, ▲ − T = 313.15 K. Reddy and Naidu[14] propan-1-ol: □ − T = 303.15 K, ○ − T = 313.15 K; butan-1-ol: ∇ − T = 308.15 K, Δ − T = 313.15 K.

from eq 2 differs from the respective experimental value by less than $5\cdot10^{-3}$ kg·m^{-3}, that is, the difference is 10 times smaller than the estimated measurement uncertainty.

Similar to the logarithm of the specific volume, the dependence of the speed of sound on temperature was approximated by the third-order polynomial:

$$u/(\mathrm{m\cdot s^{-1}}) = u_{25} + \sum_{i=1}^{3} b_i \vartheta^i \tag{3}$$

with the coefficients u_{25} and b_i obtained in the same way as those of eq 2. Speeds of sound calculated from eq 3 are equal to the measured values within the range of ±0.1 m·s^{-1}. The coefficients of eqs 2 and 3 are reported in Tables 6 and 7.

Temperature derivative of eq 2 gives the coefficient of thermal expansion at constant pressure:

$$\alpha_p \equiv V^{-1}(\partial V/\partial T)_p = \sum_{i=1}^{3} i a_i \vartheta^{i-1} \tag{4}$$

From eqs 2 and 4, the molar isobaric expansions could be calculated:

$$E_{p,\mathrm{m}} \equiv (\partial V_\mathrm{m}/\partial T)_p = \alpha_p V_\mathrm{m} \tag{5}$$

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Table 2. Experimental Densities and Speeds of Sound in the Binary System Butan-2-one (1) + Methanol (2), Isentropic Compressibilities (eq 1)[a] and Molar Excesses of Volume, Isentropic Compression, and Thermal Expansion (eq 8)

	T	ρ	u	$\kappa_S \cdot 10^{10}$	$V^E_m \cdot 10^6$	$K^E_{S,m} \cdot 10^{14}$	$E^E_{p,m} \cdot 10^9$
x_1	K	$kg \cdot m^{-3}$	$m \cdot s^{-1}$	Pa^{-1}	$m^3 \cdot mol^{-1}$	$m^3 \cdot mol^{-1} \cdot Pa^{-1}$	$m^3 \cdot mol^{-1} \cdot K^{-1}$
0	293.151	791.283	1119.30	10.0873			
0	298.149	786.577	1102.81	10.4534			
0	303.149	781.849	1086.39	10.8369			
0	308.149	777.101	1070.16	11.2363			
0	313.149	772.316	1053.93	11.6569			
0	318.149	767.513	1037.89	12.0952			
0	323.149	762.669	1021.87	12.5566			
0.0962	293.151	795.933	1142.79	9.6203	−0.1160	−0.0870	0.20
0.0962	298.149	791.075	1125.40	9.9809	−0.1143	−0.0908	0.35
0.0962	303.149	786.188	1107.98	10.3612	−0.1123	−0.0938	0.45
0.0962	308.149	781.263	1090.54	10.7627	−0.1096	−0.0958	0.52
0.0962	313.149	776.323	1073.35	11.1809	−0.1076	−0.0995	0.56
0.0962	318.149	771.341	1056.21	11.6213	−0.1048	−0.1027	0.55
0.0962	323.149	766.318	1039.12	12.0854	−0.1015	−0.1053	0.51
0.2200	293.151	799.736	1163.88	9.2307	−0.2050	−0.1456	0.23
0.2200	298.149	794.761	1145.63	9.5868	−0.2030	−0.1529	0.47
0.2200	303.149	789.746	1127.31	9.9638	−0.2001	−0.1593	0.68
0.2200	308.150	784.692	1109.04	10.3611	−0.1965	−0.1658	0.87
0.2200	313.149	779.594	1090.78	10.7810	−0.1916	−0.1715	1.02
0.2200	318.149	774.457	1072.56	11.2243	−0.1862	−0.1768	1.15
0.2200	323.149	769.280	1054.46	11.6911	−0.1801	−0.1823	1.24
0.3083	293.151	801.566	1175.12	9.0343	−0.2422	−0.1665	0.24
0.3083	298.151	796.520	1156.23	9.3911	−0.2396	−0.1741	0.52
0.3083	303.151	791.443	1137.56	9.7641	−0.2366	−0.1837	0.78
0.3083	308.151	786.319	1118.75	10.1610	−0.2323	−0.1916	1.02
0.3083	313.150	781.154	1100.00	10.5798	−0.2270	−0.1995	1.23
0.3083	318.150	775.936	1081.20	11.0246	−0.2200	−0.2060	1.42
0.3083	323.149	770.680	1062.51	11.4937	−0.2123	−0.2126	1.58
0.3858	293.151	802.742	1183.56	8.8929	−0.2593	−0.1781	0.10
0.3858	298.149	797.675	1164.26	9.2486	−0.2581	−0.1867	0.42
0.3858	303.149	792.552	1144.93	9.6253	−0.2550	−0.1947	0.73
0.3858	308.149	787.383	1125.71	10.0222	−0.2505	−0.2036	1.02
0.3858	313.149	782.172	1106.54	10.4415	−0.2451	−0.2124	1.29
0.3858	318.149	776.910	1087.37	10.8862	−0.2379	−0.2204	1.54
0.3858	323.149	771.601	1068.25	11.3569	−0.2294	−0.2279	1.77
0.4983	293.151	803.936	1193.21	8.7366	−0.2626	−0.1792	0.42
0.4983	298.149	798.805	1173.52	9.0903	−0.2603	−0.1891	0.51
0.4983	303.149	793.636	1153.77	9.4654	−0.2576	−0.1986	0.68
0.4983	308.149	788.417	1134.01	9.8630	−0.2531	−0.2079	0.93
0.4983	313.149	783.159	1114.30	10.2836	−0.2480	−0.2173	1.26
0.4983	318.149	777.848	1094.65	10.7289	−0.2408	−0.2266	1.68
0.4983	323.149	772.478	1074.91	11.2039	−0.2310	−0.2332	2.17
0.5781	293.149	804.516	1198.84	8.6485	−0.2519	−0.1727	0.69
0.5781	298.149	799.344	1178.83	9.0025	−0.2488	−0.1824	0.67
0.5781	303.149	794.136	1158.73	9.3787	−0.2451	−0.1913	0.75
0.5781	308.149	788.889	1138.70	9.7761	−0.2408	−0.2010	0.94
0.5781	313.149	783.601	1118.69	10.1973	−0.2355	−0.2106	1.24
0.5781	318.149	778.265	1098.69	10.6444	−0.2285	−0.2196	1.66
0.5781	323.149	772.868	1078.58	11.1222	−0.2186	−0.2253	2.20
0.6964	293.151	805.035	1205.53	8.5473	−0.2155	−0.1516	0.53
0.6964	298.149	799.830	1185.30	8.8991	−0.2121	−0.1624	0.73
0.6964	303.149	794.583	1164.78	9.2763	−0.2081	−0.1704	0.92
0.6964	308.149	789.292	1144.22	9.6771	−0.2028	−0.1776	1.10
0.6964	313.149	783.968	1123.78	10.1004	−0.1973	−0.1862	1.28
0.6964	318.149	778.602	1103.38	10.5496	−0.1906	−0.1944	1.44
0.6964	323.149	773.192	1083.00	11.0270	−0.1824	−0.2016	1.60
0.7943	293.151	805.218	1209.85	8.4844	−0.1666	−0.1241	0.52
0.7943	298.149	799.991	1189.19	8.8392	−0.1632	−0.1320	0.68

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Table 2. continued

x_1	T / K	ρ / kg·m^{-3}	u / m·s^{-1}	$\kappa_S \cdot 10^{10}$ / Pa^{-1}	$V_m^E \cdot 10^6$ / m^3·mol^{-1}	$K_{S,m}^E \cdot 10^{14}$ / m^3·mol^{-1}·Pa^{-1}	$E_{p,m}^E \cdot 10^9$ / m^3·mol^{-1}·K^{-1}
0.7943	303.149	794.727	1168.35	9.2180	−0.1596	−0.1383	0.84
0.7943	308.149	789.419	1147.47	9.6208	−0.1548	−0.1437	0.99
0.7943	313.149	784.079	1126.71	10.0465	−0.1499	−0.1503	1.13
0.7943	318.149	778.700	1106.00	10.4983	−0.1441	−0.1568	1.27
0.7943	323.149	773.276	1085.30	10.9791	−0.1367	−0.1617	1.41
0.8857	293.151	805.214	1212.45	8.4481	−0.1047	−0.0832	0.37
0.8857	298.149	799.977	1191.48	8.8054	−0.1019	−0.0882	0.49
0.8857	303.149	794.706	1170.36	9.1866	−0.0993	−0.0918	0.61
0.8857	308.149	789.400	1149.30	9.5904	−0.0965	−0.0960	0.73
0.8857	313.149	784.049	1128.19	10.0206	−0.0923	−0.0985	0.84
0.8857	318.149	778.666	1107.23	10.4755	−0.0879	−0.1022	0.95
0.8857	323.149	773.245	1086.29	10.9595	−0.0826	−0.1045	1.06
1	293.151	804.965	1213.15	8.4410			
1	298.149	799.739	1191.97	8.8008			
1	303.149	794.471	1170.57	9.1860			
1	308.149	789.176	1149.31	9.5929			
1	313.149	783.846	1128.08	10.0251			
1	318.149	778.481	1106.94	10.4834			
1	323.149	773.086	1085.89	10.9698			

[a]Standard uncertainties u are $u(x_1) = 5 \cdot 10^{-5}$, $u(T) = 0.05$ K, and the combined expanded uncertainties U_c are $U_c(\rho) = 0.05$ kg·m^{-3}, $U_c(u) = 0.5$ m·s^{-1}, $U_c(\kappa_S) = 1 \cdot 10^{-13}$ Pa^{-1} (0.95 level of confidence)

Table 3. Experimental Densities and Speeds of Sound in the Binary System Butan-2-one (1) + Propan-1-ol (2), Isentropic Compressibilities (eq 1)[a] and Molar Excesses of Volume, Isentropic Compression, and Thermal Expansion (eq 8)

x_1	T / K	ρ / kg·m^{-3}	u / m·s^{-1}	$\kappa_S \cdot 10^{10}$ / Pa^{-1}	$V_m^E \cdot 10^6$ / m^3·mol^{-1}	$K_{S,m}^E \cdot 10^{14}$ / m^3·mol^{-1}·Pa^{-1}	$E_{p,m}^E \cdot 10^9$ / m^3·mol^{-1}·K^{-1}
0	293.151	803.476	1222.55	8.3271			
0	298.153	799.471	1205.64	8.6052			
0	303.154	795.437	1188.77	8.8961			
0	308.155	791.372	1172.01	9.1993			
0	313.154	787.262	1155.35	9.5160			
0	318.155	783.104	1138.65	9.8492			
0	323.155	778.897	1121.93	10.1997			
0.0715	293.154	803.777	1223.57	8.3101	−0.0178	−0.0350	0.74
0.0715	298.154	799.630	1206.22	8.5952	−0.0142	−0.0369	0.79
0.0715	303.154	795.449	1188.64	8.8979	−0.0100	−0.0352	0.82
0.0715	308.154	791.232	1171.17	9.2142	−0.0057	−0.0336	0.84
0.0715	313.154	786.978	1153.83	9.5445	−0.0016	−0.0329	0.84
0.0715	318.156	782.677	1136.56	9.8908	0.0024	−0.0331	0.83
0.0715	323.156	778.324	1119.36	10.2542	0.0067	−0.0342	0.80
0.2005	293.153	804.182	1223.86	8.3020	−0.0381	−0.0747	1.62
0.2005	298.154	799.805	1205.46	8.6042	−0.0298	−0.0752	1.71
0.2005	303.154	795.395	1187.12	8.9213	−0.0210	−0.0752	1.79
0.2005	308.155	790.950	1168.90	9.2533	−0.0119	−0.0759	1.85
0.2005	313.155	786.464	1150.81	9.6009	−0.0025	−0.0776	1.89
0.2005	318.154	781.936	1132.85	9.9652	0.0069	−0.0810	1.92
0.2005	323.155	777.356	1115.06	10.3463	0.0166	−0.0874	1.93
0.3006	293.151	804.352	1223.04	8.3114	−0.0408	−0.0873	2.07
0.3006	298.153	799.821	1204.22	8.6218	−0.0305	−0.0897	2.11
0.3006	303.154	795.256	1185.39	8.9489	−0.0195	−0.0911	2.16
0.3006	308.155	790.663	1166.65	9.2924	−0.0088	−0.0930	2.23
0.3006	313.155	786.028	1147.98	9.6537	0.0025	−0.0953	2.31
0.3006	318.155	781.346	1129.37	10.0342	0.0145	−0.0981	2.41
0.3006	323.155	776.616	1110.82	10.4353	0.0267	−0.1020	2.52
0.3996	293.152	804.467	1221.91	8.3256	−0.0390	−0.0913	2.15
0.3996	298.153	799.804	1202.65	8.6445	−0.0281	−0.0944	2.29
0.3996	303.155	795.106	1183.46	8.9798	−0.0163	−0.0978	2.41
0.3996	308.155	790.370	1164.31	9.3332	−0.0036	−0.1009	2.52
0.3996	313.154	785.600	1145.23	9.7054	0.0090	−0.1048	2.61

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Table 3. continued

x_1	T / K	ρ / kg·m^{-3}	u / m·s^{-1}	$\kappa_S \cdot 10^{10}$ / Pa^{-1}	$V_m^E \cdot 10^6$ / m^3·mol^{-1}	$K_{S,m}^E \cdot 10^{14}$ / m^3·mol^{-1}·Pa^{-1}	$E_{p,m}^E \cdot 10^9$ / m^3·mol^{-1}·K^{-1}
0.3996	318.155	780.785	1126.21	10.0979	0.0220	−0.1095	2.68
0.3996	323.155	775.920	1107.24	10.5123	0.0358	−0.1150	2.73
0.5024	293.152	804.599	1220.74	8.3402	−0.0388	−0.0910	1.83
0.5024	298.154	799.814	1201.25	8.6645	−0.0284	−0.0971	2.22
0.5024	303.154	794.989	1181.62	9.0091	−0.0163	−0.1009	2.51
0.5024	308.154	790.125	1162.06	9.3723	−0.0033	−0.1051	2.69
0.5024	313.154	785.227	1142.57	9.7553	0.0097	−0.1101	2.76
0.5024	318.155	780.284	1123.14	10.1597	0.0234	−0.1159	2.73
0.5024	323.156	775.293	1103.75	10.5875	0.0377	−0.1224	2.59
0.5993	293.153	804.707	1219.89	8.3507	−0.0375	−0.0893	2.01
0.5993	298.153	799.809	1199.95	8.6834	−0.0270	−0.0947	2.18
0.5993	303.154	794.877	1180.01	9.0350	−0.0157	−0.0997	2.35
0.5993	308.154	789.907	1160.11	9.4064	−0.0035	−0.1049	2.51
0.5993	313.154	784.898	1140.29	9.7984	0.0094	−0.1109	2.67
0.5993	318.155	779.842	1120.50	10.2134	0.0233	−0.1172	2.83
0.5993	323.155	774.741	1100.75	10.6529	0.0378	−0.1242	2.99
0.6994	293.152	804.703	1218.82	8.3654	−0.0241	−0.0792	1.77
0.6994	298.153	799.703	1198.45	8.7063	−0.0148	−0.0836	1.95
0.6994	303.154	794.670	1178.10	9.0667	−0.0048	−0.0878	2.11
0.6994	308.154	789.597	1157.82	9.4474	0.0065	−0.0922	2.24
0.6994	313.154	784.493	1137.61	9.8497	0.0176	−0.0975	2.36
0.6994	318.156	779.342	1117.43	10.2762	0.0297	−0.1030	2.46
0.6994	323.156	774.150	1097.31	10.7279	0.0423	−0.1091	2.53
0.7995	293.152	804.771	1217.75	8.3794	−0.0185	−0.0664	1.17
0.7995	298.154	799.680	1197.05	8.7269	−0.0114	−0.0705	1.49
0.7995	303.154	794.556	1176.35	9.0950	−0.0034	−0.0739	1.73
0.7995	308.154	789.393	1155.72	9.4842	0.0058	−0.0776	1.87
0.7995	313.154	784.201	1135.15	9.8961	0.0147	−0.0817	1.92
0.7995	318.155	778.968	1114.61	10.3332	0.0241	−0.0859	1.87
0.7995	323.155	773.693	1094.15	10.7964	0.0340	−0.0907	1.73
0.8990	293.152	804.821	1215.98	8.4033	−0.0113	−0.0409	0.87
0.8990	298.154	799.650	1194.93	8.7582	−0.0071	−0.0432	0.93
0.8990	303.154	794.445	1173.85	9.1351	−0.0018	−0.0441	0.99
0.8990	308.155	789.215	1152.85	9.5336	0.0030	−0.0454	1.05
0.8990	313.154	783.949	1131.94	9.9556	0.0085	−0.0470	1.10
0.8990	318.155	778.645	1111.10	10.4029	0.0141	−0.0489	1.15
0.8990	323.156	773.301	1090.29	10.8785	0.0200	−0.0505	1.19
1	293.152	804.834	1213.35	8.4396			
1	298.155	799.597	1192.06	8.8010			
1	303.154	794.334	1170.77	9.1845			
1	308.154	789.044	1149.56	9.5904			
1	313.154	783.720	1128.44	10.0203			
1	318.155	778.362	1107.39	10.4765			
1	323.155	772.966	1086.41	10.9610			

[a]Standard uncertainties u are $u(x_1) = 5 \cdot 10^{-5}$, $u(T) = 0.05$ K, and the combined expanded uncertainties U_c are $U_c(\rho) = 0.05$ kg·m^{-3}, $U_c(u) = 0.5$ m·s^{-1}, $U_c(\kappa_S) = 1 \cdot 10^{-13}$ Pa^{-1} (0.95 level of confidence).

where V_m is the molar volume of the system:

$$V_m = (x_1 M_1 + x_2 M_2)\nu \quad (6)$$

x is the mole fraction, and M is the molar mass, subscripts 1 and 2 denote the binary mixture components. In this work "1" stands for butan-2-one and "2" for methanol, ethanol, propan-1-ol, butan-1-ol, or chloroform.

A formula similar to eq 5 is valid for the molar isentropic compression:

$$K_{S,m} \equiv -(\partial V_m/\partial p)_S = \kappa_S V_m \quad (7)$$

where κ_S is given by eq 1.

Thermodynamic excesses of the molar volume, expansion, and isentropic compression were calculated from the definition:

$$Z_m^E = Z_m - Z_m^{id} \quad (8)$$

where $Z = V$, E_p, or K_S, and the superscript "id" denotes the ideal mixture. For V (eq 6) and E_p (eq 5):

$$Z_m^{id} = x_1 Z_1^0 + x_2 Z_2^0 \quad (9)$$

where the functions marked with "0" in the superscript are the molar quantities for the pure substances.

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Table 4. Experimental Densities and Speeds of Sound in the Binary System Butan-2-one (1) + Butan-1-ol (2), Isentropic Compressibilities (eq 1)[a] and Molar Excesses of Volume, Isentropic Compression, and Thermal Expansion (eq 8)

	T	ρ	u	$\kappa_S \cdot 10^{10}$	$V^E_m \cdot 10^6$	$K^E_{S,m} \cdot 10^{14}$	$E^E_{p,m} \cdot 10^9$
x_1	K	$kg \cdot m^{-3}$	$m \cdot s^{-1}$	Pa^{-1}	$m^3 \cdot mol^{-1}$	$m^3 \cdot mol^{-1} \cdot Pa^{-1}$	$m^3 \cdot mol^{-1} \cdot K^{-1}$
0	293.151	809.613	1257.01	7.8171			
0	298.149	805.808	1240.37	8.0661			
0	303.149	801.969	1223.64	8.3279			
0	308.149	798.101	1206.95	8.6013			
0	313.149	794.193	1190.34	8.8865			
0	318.149	790.244	1173.84	9.1838			
0	323.149	786.250	1157.36	9.4952			
0.1033	293.151	809.161	1253.19	7.8692	−0.0028	−0.0351	0.91
0.1033	298.150	805.170	1235.96	8.1302	0.0016	−0.0380	0.88
0.1033	303.149	801.150	1218.60	8.4055	0.0060	−0.0396	0.85
0.1033	308.149	797.099	1201.30	8.6933	0.0102	−0.0425	0.82
0.1033	313.149	793.012	1184.11	8.9937	0.0142	−0.0474	0.79
0.1033	318.149	788.886	1166.99	9.3079	0.0180	−0.0540	0.75
0.1033	323.149	784.717	1149.96	9.6365	0.0217	−0.0628	0.72
0.2069	293.151	808.682	1248.52	7.9329	−0.0030	−0.0549	1.49
0.2069	298.151	804.522	1230.78	8.2054	0.0039	−0.0599	1.38
0.2069	303.150	800.336	1212.91	8.4932	0.0106	−0.0641	1.33
0.2069	308.150	796.113	1195.07	8.7951	0.0177	−0.0695	1.34
0.2069	313.151	791.857	1177.32	9.1110	0.0244	−0.0771	1.41
0.2069	318.149	787.562	1159.64	9.4421	0.0312	−0.0866	1.54
0.2069	323.149	783.207	1141.75	9.7945	0.0399	−0.0936	1.74
0.3055	293.151	808.213	1243.90	7.9966	−0.0019	−0.0658	1.72
0.3055	298.151	803.902	1225.51	8.2825	0.0064	−0.0701	1.68
0.3055	303.151	799.560	1207.32	8.5803	0.0149	−0.0779	1.65
0.3055	308.150	795.189	1189.09	8.8941	0.0231	−0.0864	1.63
0.3055	313.151	790.782	1170.90	9.2237	0.0312	−0.0969	1.61
0.3055	318.150	786.339	1152.79	9.5695	0.0391	−0.1099	1.61
0.3055	323.149	781.851	1134.72	9.9334	0.0473	−0.1250	1.61
0.3998	293.151	807.770	1239.61	8.0564	−0.0017	−0.0726	1.71
0.3998	298.151	803.322	1221.08	8.3488	0.0070	−0.0817	1.78
0.3998	303.150	798.841	1202.31	8.6598	0.0162	−0.0890	1.82
0.3998	308.151	794.328	1183.64	8.9859	0.0252	−0.0992	1.84
0.3998	313.150	789.780	1165.03	9.3287	0.0343	−0.1115	1.82
0.3998	318.150	785.192	1146.45	9.6898	0.0435	−0.1259	1.78
0.3998	323.150	780.568	1127.99	10.0688	0.0521	−0.1441	1.71
0.5002	293.151	807.329	1235.42	8.1156	−0.0051	−0.0792	1.73
0.5002	298.149	802.740	1216.38	8.4195	0.0035	−0.0883	1.79
0.5002	303.149	798.114	1197.20	8.7418	0.0129	−0.0972	1.83
0.5002	308.149	793.459	1178.15	9.0798	0.0218	−0.1094	1.85
0.5002	313.149	788.765	1159.11	9.4363	0.0313	−0.1233	1.85
0.5002	318.149	784.037	1140.14	9.8118	0.0403	−0.1402	1.82
0.5002	323.149	779.268	1121.21	10.2080	0.0494	−0.1595	1.77
0.5937	293.151	806.880	1231.47	8.1723	−0.0043	−0.0787	1.57
0.5937	298.150	802.161	1212.18	8.4841	0.0039	−0.0901	1.65
0.5937	303.149	797.412	1192.70	8.8157	0.0122	−0.1008	1.69
0.5937	308.150	792.628	1173.24	9.1655	0.0206	−0.1135	1.71
0.5937	313.150	787.807	1153.82	9.5346	0.0293	−0.1283	1.69
0.5937	318.150	782.953	1134.49	9.9235	0.0376	−0.1465	1.65
0.5937	323.150	778.061	1115.23	10.3337	0.0457	−0.1677	1.58
0.7008	293.151	806.418	1227.47	8.2303	−0.0094	−0.0789	1.39
0.7008	298.151	801.555	1207.71	8.5535	−0.0024	−0.0901	1.45
0.7008	303.150	796.660	1187.75	8.8977	0.0050	−0.1002	1.49
0.7008	308.150	791.730	1167.81	9.2614	0.0127	−0.1121	1.53
0.7008	313.150	786.766	1147.93	9.6455	0.0203	−0.1264	1.55
0.7008	318.150	781.765	1128.12	10.0511	0.0280	−0.1433	1.55
0.7008	323.149	776.725	1108.31	10.4812	0.0358	−0.1616	1.54
0.8030	293.151	805.915	1223.62	8.2874	−0.0075	−0.0709	0.90
0.8030	298.149	800.920	1203.33	8.6227	−0.0019	−0.0796	1.11

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Table 4. continued

x_1	T / K	ρ / kg·m^{-3}	u / m·s^{-1}	$\kappa_S \cdot 10^{10}$ / Pa^{-1}	$V^E_m \cdot 10^6$ / m^3·mol^{-1}	$K^E_{S,m} \cdot 10^{14}$ / m^3·mol^{-1}·Pa^{-1}	$E^E_{p,m} \cdot 10^9$ / m^3·mol^{-1}·K^{-1}
0.8030	303.149	795.887	1182.84	8.9804	0.0045	−0.0870	1.26
0.8030	308.149	790.827	1162.46	9.3576	0.0102	−0.0971	1.33
0.8030	313.149	785.725	1142.04	9.7581	0.0170	−0.1074	1.33
0.8030	318.149	780.596	1121.75	10.1808	0.0227	−0.1208	1.26
0.8030	323.149	775.415	1101.39	10.6312	0.0301	−0.1334	1.12
0.8974	293.151	805.458	1219.34	8.3504	−0.0069	−0.0488	0.77
0.8974	298.151	800.340	1198.40	8.7001	−0.0029	−0.0519	0.73
0.8974	303.151	795.198	1177.74	9.0662	0.0004	−0.0597	0.71
0.8974	308.151	790.021	1156.89	9.4575	0.0040	−0.0653	0.70
0.8974	313.151	784.812	1136.08	9.8723	0.0075	−0.0720	0.71
0.8974	318.151	779.565	1115.34	10.3118	0.0113	−0.0798	0.74
0.8974	323.149	774.284	1094.68	10.7777	0.0150	−0.0887	0.79
1	293.151	804.903	1213.30	8.4396			
1	298.149	799.678	1192.14	8.7989			
1	303.149	794.414	1170.79	9.1832			
1	308.149	789.124	1149.57	9.5892			
1	313.149	783.798	1128.37	10.0206			
1	318.149	778.438	1107.27	10.4778			
1	323.149	773.040	1086.19	10.9644			

[a]Standard uncertainties u are $u(x_1) = 5 \cdot 10^{-5}$, $u(T) = 0.05$ K, and the combined expanded uncertainties U_c are $U_c(\rho) = 0.05$ kg·m^{-3}, $U_c(u) = 0.5$ m·s^{-1}, $U_c(\kappa_S) = 1 \cdot 10^{-13}$ Pa^{-1} (0.95 level of confidence).

Table 5. Experimental Densities and Speeds of Sound in the Binary System Butan-2-one (1) + Chloroform (2), Isentropic Compressibilities (eq 1)[a] and Molar Excesses of Volume, Isentropic Compression, and Thermal Expansion (eq 8)

x_1	T / K	ρ / kg·m^{-3}	u / m·s^{-1}	$\kappa_S \cdot 10^{10}$ / Pa^{-1}	$V^E_m \cdot 10^6$ / m^3·mol^{-1}	$K^E_{S,m} \cdot 10^{14}$ / m^3·mol^{-1}·Pa^{-1}	$E^E_{p,m} \cdot 10^9$ / m^3·mol^{-1}·K^{-1}
0	293.151	1487.632	1000.63	6.7136			
0	298.149	1478.156	983.68	6.9915			
0	303.149	1468.608	966.68	7.2867			
0	308.149	1459.003	949.78	7.5980			
0.0985	293.151	1414.988	1010.23	6.9248	−0.0876	0.0035	−0.93
0.0985	298.149	1406.027	993.35	7.2078	−0.0924	−0.0001	−1.00
0.0985	303.149	1397.007	976.36	7.5090	−0.0976	−0.0032	−1.07
0.0985	308.149	1387.933	959.40	7.8277	−0.1032	−0.0074	−1.15
0.1786	293.151	1356.752	1018.87	7.1001	−0.1439	0.0152	−2.73
0.1786	298.149	1348.262	1002.10	7.3859	−0.1563	0.0076	−2.53
0.1786	303.149	1339.723	985.21	7.6900	−0.1696	−0.0002	−2.33
0.1786	308.150	1331.074	968.21	8.0142	−0.1800	−0.0075	−2.12
0.3051	293.151	1266.117	1037.47	7.3663	−0.1911	0.0366	−3.22
0.3051	298.151	1258.189	1020.08	7.6381	−0.2052	0.0080	−2.91
0.3051	303.151	1250.227	1002.87	7.9528	−0.2209	−0.0010	−2.60
0.3051	308.151	1242.140	985.85	8.2834	−0.2318	−0.0137	−2.28
0.3895	293.151	1206.738	1051.13	7.5002	−0.2039	0.0213	−2.94
0.3895	298.149	1199.182	1033.90	7.8011	−0.2189	0.0111	−3.04
0.3895	303.149	1191.573	1016.54	8.1214	−0.2342	0.0004	−3.14
0.3895	308.149	1183.921	999.24	8.4594	−0.2503	−0.0134	−3.24
0.5205	293.151	1116.203	1076.15	7.7359	−0.1848	0.0313	−3.28
0.5205	298.149	1109.214	1058.53	8.0460	−0.2013	0.0201	−3.34
0.5205	303.149	1102.177	1040.71	8.3770	−0.2182	0.0091	−3.40
0.5205	308.149	1095.095	1022.92	8.7270	−0.2354	−0.0050	−3.47
0.6356	293.151	1038.571	1102.27	7.9248	−0.1483	0.0337	−3.05
0.6356	298.149	1032.041	1084.03	8.2456	−0.1638	0.0244	−3.10
0.6356	303.149	1025.464	1065.59	8.5881	−0.1793	0.0155	−3.15
0.6356	308.149	1018.848	1047.20	8.9502	−0.1953	0.0032	−3.20
0.7219	293.151	981.684	1124.50	8.0558	−0.1228	0.0305	−2.60
0.7219	298.149	975.475	1105.69	8.3853	−0.1359	0.0235	−2.64
0.7219	303.149	969.225	1086.69	8.7370	−0.1492	0.0169	−2.68
0.7219	308.149	962.936	1067.73	9.1092	−0.1627	0.0074	−2.72
0.7939	293.151	934.854	1144.89	8.1607	−0.0835	0.0280	−2.24

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Table 5. continued

x_1	T / K	ρ / kg·m^{-3}	u / m·s^{-1}	$\kappa_S \cdot 10^{10}$ / Pa^{-1}	$V^E_m \cdot 10^6$ / m^3·mol^{-1}	$K^E_{S,m} \cdot 10^{14}$ / m^3·mol^{-1}·Pa^{-1}	$E^E_{p,m} \cdot 10^9$ / m^3·mol^{-1}·K^{-1}
0.7939	298.149	928.929	1125.37	8.5002	−0.0960	0.0254	−2.04
0.7939	303.149	922.905	1105.87	8.8600	−0.1029	0.0218	−1.84
0.7939	308.149	916.881	1086.53	9.2385	−0.1134	0.0131	−1.64
0.8539	293.151	896.434	1163.45	8.2411	−0.0535	0.0212	−1.53
0.8539	298.149	890.699	1143.51	8.5860	−0.0612	0.0203	−1.53
0.8539	303.149	884.925	1123.49	8.9527	−0.0688	0.0188	−1.53
0.8539	308.149	879.117	1103.56	9.3403	−0.0765	0.0143	−1.53
0.9089	293.151	861.829	1181.36	8.3141	−0.0431	0.0143	−1.01
0.9089	298.149	856.285	1161.02	8.6637	−0.0481	0.0144	−1.00
0.9089	303.149	850.704	1140.53	9.0367	−0.0531	0.0152	−1.00
0.9089	308.149	845.091	1120.11	9.4314	−0.0581	0.0135	−0.99
1	293.151	805.166	1214.03	8.4267			
1	298.149	799.937	1193.15	8.7812			
1	303.149	794.672	1172.10	9.1597			
1	308.149	789.382	1151.00	9.5623			

[a]Standard uncertainties u are $u(x_1) = 5 \cdot 10^{-5}$, $u(T) = 0.05$ K, and the combined expanded uncertainties U_c are $U_c(\rho) = 0.05$ kg·m^{-3}, $U_c(u) = 0.5$ m·s^{-1}, $U_c(\kappa_S) = 1 \cdot 10^{-13}$ Pa^{-1} (0.95 level of confidence).

Table 6. Coefficients of eq 2 for the Specific Volume of Binary Systems Butan-2-one (1) + Cosolvent (2) and Standard Errors of the Fit (δ)

cosolvent	x_1	ln v_{25}	$a_1 \cdot 10^3$	$a_2 \cdot 10^6$	$a_3 \cdot 10^8$	δ
CH_3OH	0	0.2400653 ± 0.0000026	1.19937 ± 0.00045	1.240 ± 0.064	0.69 ± 0.21	3.8
	0.0962	0.2343607 ± 0.0000042	1.23159 ± 0.00075	1.604 ± 0.034		7.9
	0.2200	0.2297120 ± 0.0000016	1.25676 ± 0.00028	1.871 ± 0.013		2.9
	0.3083	0.2274937 ± 0.0000034	1.27010 ± 0.00060	1.975 ± 0.027		6.3
	0.3858	0.2260569 ± 0.0000016	1.27754 ± 0.00028	2.067 ± 0.013		2.9
	0.4983	0.2246396 ± 0.0000020	1.28980 ± 0.00034	1.785 ± 0.049	0.97 ± 0.16	2.9
	0.5781	0.2239671 ± 0.0000017	1.29844 ± 0.00030	1.653 ± 0.043	1.19 ± 0.14	2.6
	0.6964	0.2233563 ± 0.0000018	1.30690 ± 0.00032	1.916 ± 0.015		3.4
	0.7943	0.2231534 ± 0.0000022	1.31145 ± 0.00039	1.884 ± 0.018		4.1
	0.8857	0.2231692 ± 0.0000020	1.31328 ± 0.00035	1.853 ± 0.016		3.7
	1	0.2234724 ± 0.0000012	1.31208 ± 0.00022	1.746 ± 0.010		2.3
C_3H_7OH	0	0.2238017 ± 0.0000014	1.00478 ± 0.00024	1.236 ± 0.034	1.14 ± 0.11	2.0
	0.0715	0.2236038 ± 0.0000014	1.04136 ± 0.00025	1.306 ± 0.036	0.97 ± 0.11	2.1
	0.2005	0.2233837 ± 0.0000006	1.09829 ± 0.00010	1.398 ± 0.014	0.87 ± 0.05	0.8
	0.3006	0.2233659 ± 0.0000015	1.13645 ± 0.00026	1.373 ± 0.037	1.07 ± 0.12	2.2
	0.3996	0.2233861 ± 0.0000016	1.17009 ± 0.00027	1.510 ± 0.039	0.75 ± 0.13	2.3
	0.5024	0.2233704 ± 0.0000029	1.20070 ± 0.00051	1.782 ± 0.023		5.4
	0.5993	0.2233783 ± 0.0000005	1.22880 ± 0.00008	1.604 ± 0.011	0.76 ± 0.04	0.7
	0.6994	0.2235114 ± 0.0000015	1.25443 ± 0.00027	1.627 ± 0.038	0.59 ± 0.12	2.3
	0.7995	0.2235366 ± 0.0000026	1.27671 ± 0.00046	1.783 ± 0.021		4.8
	0.8990	0.2235787 ± 0.0000016	1.29697 ± 0.00028	1.560 ± 0.041	0.64 ± 0.13	2.4
	1	0.2236423 ± 0.0000009	1.31269 ± 0.00015	1.526 ± 0.022	0.64 ± 0.07	1.3
C_4H_9OH	0	0.2159119 ± 0.0000009	0.94850 ± 0.00015	1.170 ± 0.022	0.81 ± 0.07	1.3
	0.1033	0.2167024 ± 0.0000003	0.99494 ± 0.00005	1.181 ± 0.008	0.76 ± 0.02	0.4
	0.2069	0.2175073 ± 0.0000023	1.03749 ± 0.00041	1.168 ± 0.059	1.17 ± 0.19	3.5
	0.3055	0.2182784 ± 0.0000010	1.07622 ± 0.00017	1.263 ± 0.025	0.76 ± 0.08	1.5
	0.3998	0.2189992 ± 0.0000009	1.11141 ± 0.00016	1.404 ± 0.023	0.46 ± 0.07	1.3
	0.5002	0.2197269 ± 0.0000010	1.14798 ± 0.00018	1.444 ± 0.026	0.46 ± 0.08	1.5
	0.5937	0.2204450 ± 0.0000008	1.18045 ± 0.00015	1.494 ± 0.021	0.39 ± 0.07	1.3
	0.7008	0.2212011 ± 0.0000005	1.21747 ± 0.00009	1.537 ± 0.013	0.46 ± 0.04	0.8
	0.8030	0.2219932 ± 0.0000037	1.25133 ± 0.00065	1.721 ± 0.030		6.9
	0.8974	0.2227156 ± 0.0000011	1.28192 ± 0.00018	1.535 ± 0.027	0.61 ± 0.09	1.6
	1	0.2235500 ± 0.0000014	1.31170 ± 0.00025	1.620 ± 0.036	0.45 ± 0.11	2.1
$CHCl_3$	0	−0.3907931 ± 0.0000010	1.28725 ± 0.00019	1.689 ± 0.028		1.4
	0.0985	−0.3407668 ± 0.0000000	1.27915 ± 0.00001	1.609 ± 0.001		0.1
	0.1786	−0.2988223 ± 0.0000080	1.26381 ± 0.00145	1.957 ± 0.216		10.8
	0.3051	−0.2296858 ± 0.0000123	1.26370 ± 0.00223	2.081 ± 0.332		16.6
	0.3895	−0.1816377 ± 0.0000008	1.26486 ± 0.00014	1.588 ± 0.021		1.0

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Table 6. continued

cosolvent	x_1	ln v_{25}	$a_1 \cdot 10^3$	$a_2 \cdot 10^6$	$a_3 \cdot 10^8$	δ
	0.5205	−0.1036506 ± 0.0000002	1.26481 ± 0.00003	1.626 ± 0.005		0.2
	0.6356	−0.0315365 ± 0.0000007	1.27027 ± 0.00012	1.628 ± 0.018		0.9
	0.7219	0.0248318 ± 0.0000003	1.27754 ± 0.00005	1.624 ± 0.008		0.4
	0.7939	0.0737397 ± 0.0000170	1.28564 ± 0.00309	1.880 ± 0.460		23.0
	0.8539	0.1157503 ± 0.0000003	1.29242 ± 0.00005	1.642 ± 0.008		0.4
	0.9089	0.1551536 ± 0.0000003	1.29950 ± 0.00006	1.638 ± 0.009		0.4
	0.9564	0.1902487 ± 0.0000005	1.30586 ± 0.00010	1.687 ± 0.015		0.7
	1	0.2232251 ± 0.0000016	1.31207 ± 0.00030	1.610 ± 0.044		2.2

Table 7. Coefficients of the Speed of Sound Polynomials (eq 3) for Binary Systems Butan-2-one (1) + Cosolvent (2) and Standard Errors of the Fit (δ)

cosolvent	x_1	u_{25}	b_1	$b_2 \cdot 10^3$	$b_3 \cdot 10^5$	δ
CH_3OH	0	1102.81 ± 0.01	−3.2880 ± 0.0025	2.040 ± 0.116		0.03
	0.0962	1125.38 ± 0.03	−3.4826 ± 0.0038		5.30 ± 0.69	0.05
	0.2200	1145.61 ± 0.01	−3.6600 ± 0.0015		2.17 ± 0.28	0.02
	0.3083	1156.30 ± 0.03	−3.7535 ± 0.0018			0.05
	0.3858	1164.24 ± 0.01	−3.8612 ± 0.0019	0.876 ± 0.087		0.02
	0.4983	1173.49 ± 0.02	−3.9438 ± 0.0012			0.03
	0.5781	1178.80 ± 0.02	−4.0079 ± 0.0012			0.03
	0.6964	1185.17 ± 0.04	−4.0890 ± 0.0032			0.08
	0.7943	1189.10 ± 0.04	−4.1550 ± 0.0027			0.07
	0.8857	1191.41 ± 0.04	−4.2084 ± 0.0025			0.07
	1	1191.89 ± 0.02	−4.2616 ± 0.0034		3.41 ± 0.62	0.04
C_3H_7OH	0	1205.62 ± 0.02	−3.3757 ± 0.0029	2.285 ± 0.412	−4.51 ± 1.33	0.02
	0.0715	1206.15 ± 0.03	−3.4967 ± 0.0042		4.23 ± 0.77	0.05
	0.2005	1205.47 ± 0.01	−3.6738 ± 0.0009	1.644 ± 0.130	2.75 ± 0.42	0.01
	0.3006	1204.20 ± 0.01	−3.7648 ± 0.0015	1.203 ± 0.071		0.02
	0.3996	1202.67 ± 0.00	−3.8448 ± 0.0006	1.140 ± 0.026		0.01
	0.5024	1201.21 ± 0.02	−3.9141 ± 0.0026		2.70 ± 0.48	0.03
	0.5993	1199.94 ± 0.01	−3.9891 ± 0.0013	0.886 ± 0.058		0.01
	0.6994	1198.45 ± 0.00	−4.0712 ± 0.0008	1.066 ± 0.037		0.01
	0.7995	1197.04 ± 0.01	−4.1402 ± 0.0014	0.999 ± 0.062		0.01
	0.8990	1194.91 ± 0.01	−4.2143 ± 0.0024	1.220 ± 0.109		0.02
	1	1192.05 ± 0.01	−4.2595 ± 0.0021	1.385 ± 0.095		0.02
C_4H_9OH	0	1240.33 ± 0.01	−3.3401 ± 0.0021		3.43 ± 0.38	0.03
	0.1033	1235.91 ± 0.02	−3.4628 ± 0.0024		3.97 ± 0.45	0.03
	0.2069	1230.73 ± 0.03	−3.5587 ± 0.0022			0.06
	0.3055	1225.57 ± 0.02	−3.6584 ± 0.0030	0.980 ± 0.137		0.03
	0.3998	1220.99 ± 0.03	−3.7365 ± 0.0042		2.54 ± 0.78	0.06
	0.5002	1216.33 ± 0.02	−3.8212 ± 0.0023		2.62 ± 0.42	0.03
	0.5937	1212.14 ± 0.02	−3.8792 ± 0.0036	−1.667 ± 0.524	7.16 ± 1.69	0.03
	0.7008	1207.62 ± 0.03	−3.9751 ± 0.0024			0.06
	0.8030	1203.25 ± 0.03	−4.0762 ± 0.0021			0.05
	0.8974	1198.48 ± 0.04	−4.1556 ± 0.0028			0.07
	1	1192.07 ± 0.02	−4.2528 ± 0.0030		2.82 ± 0.56	0.04
$CHCl_3$	0	983.67 ± 0.02	−3.3914 ± 0.0027			0.03
	0.0985	993.31 ± 0.02	−3.3900 ± 0.0030			0.03
	0.1786	1002.10 ± 0.00	−3.3666 ± 0.0002	−0.002 ± 0.000		0.00
	0.3051	1020.08 ± 0.00	−3.4599 ± 0.0003	0.004 ± 0.000		0.00
	0.3895	1033.85 ± 0.02	−3.4610 ± 0.0033			0.04
	0.5205	1058.45 ± 0.04	−3.5506 ± 0.0060			0.07
	0.6356	1083.95 ± 0.03	−3.6734 ± 0.0057			0.06
	0.7219	1105.62 ± 0.03	−3.7867 ± 0.0055			0.06
	0.7939	1125.35 ± 0.02	−3.9015 ± 0.0040	0.002 ± 0.001		0.03
	0.8539	1143.49 ± 0.01	−3.9943 ± 0.0024			0.03
	0.9089	1160.97 ± 0.02	−4.0853 ± 0.0038			0.04
	0.9564	1177.07 ± 0.03	−4.1707 ± 0.0045			0.05
	1	1193.13 ± 0.02	−4.1927 ± 0.0034	−0.002 ± 0.000		0.02

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Table 8. Coefficients of the Modified Redlich-Kister Polynomials (eq 11), Characteristics of the Fit: Correlation Coefficients (r) and Standard Errors of Fitting (δ), and Number of Experimental Points (n)

	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH	$CHCl_3$
			V_m^E		
a_{00}	−1.045 ± 0.001		−0.109 ± 0.003	0.020 ± 0.002	−0.813 ± 0.006
$a_{01}\cdot10^2$	0.227 ± 0.010		0.934 ± 0.035	0.713 ± 0.013	−1.290 ± 0.095
$a_{02}\cdot10^4$	0.989 ± 0.041		0.468 ± 0.146		
$a_{10}\cdot10$	−1.498 ± 0.022		−0.805 ± 0.024	0.339 ± 0.022	−4.431 ± 0.247
$a_{11}\cdot10^3$	−0.580 ± 0.132			0.658 ± 0.152	
a_{12}					
a_{20}	−0.114 ± 0.006		−0.046 ± 0.007	−0.044 ± 0.005	
$a_{21}\cdot10^2$	0.347 ± 0.016		0.250 ± 0.050		
$a_{22}\cdot10^3$				0.183 ± 0.043	
$a_{30}\cdot10$	−0.531 ± 0.044				1.705 ± 0.414
a_{31}					
$a_{32}\cdot10^4$	−0.458 ± 0.121				
a_{40}	−0.108 ± 0.009				
$a_{41}\cdot10^2$				0.396 ± 0.108	
$a_{42}\cdot10^3$				−0.332 ± 0.087	
r	0.9997		0.9968	0.9974	0.9879
δ	0.0028		0.0100	0.0062	0.0352
n	63		63	63	44
			$K_{S,m}^E$		
a_{00}	−0.754 ± 0.001	−0.477 ± 0.018	−0.386 ± 0.003	−0.345 ± 0.002	0.072 ± 0.005
$a_{01}\cdot10^2$	−0.813 ± 0.012	5.254 ± 0.272	−0.377 ± 0.021	−0.747 ± 0.020	−0.946 ± 0.076
$a_{02}\cdot10^4$	0.036 ± 0.005	−4.010 ± 0.704		−0.178 ± 0.011	
$a_{10}\cdot10$	−0.726 ± 0.029	−0.898 ± 0.137	−0.261 ± 0.034	1.115 ± 0.022	−1.037 ± 0.063
$a_{11}\cdot10^3$	0.822 ± 0.168		2.402 ± 0.243	5.104 ± 0.264	
a_{12}					
a_{20}	−0.255 ± 0.008	−0.350 ± 0.028	−0.170 ± 0.007	−0.228 ± 0.005	
$a_{21}\cdot10^2$			0.502 ± 0.095		
$a_{22}\cdot10^3$			−0.365 ± 0.064	0.167 ± 0.047	
$a_{30}\cdot10$	−0.363 ± 0.057				
$a_{31}\cdot10$		−0.329 ± 0.052			−0.098 ± 0.019
$a_{32}\cdot10^4$	−0.633 ± 0.156			−1.384 ± 0.227	
$a_{40}\cdot10$	−0.969 ± 0.122				0.887 ± 0.166
$a_{41}\cdot10^2$	0.116 ± 0.030	7.282 ± 0.806			1.401 ± 0.293
$a_{42}\cdot10^3$			0.446 ± 0.085	−0.381 ± 0.069	
r	0.9996	0.9915	0.9824	0.9992	0.9786
δ	0.0036	0.0477	0.0100	0.0064	0.0210
n	63	33	63	63	44

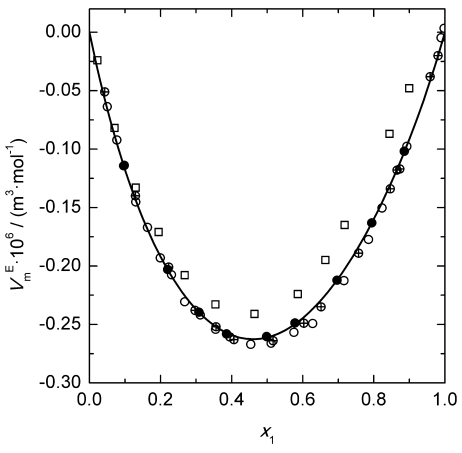

Figure 7. Excess molar volume of butan-2-one (1) + methanol (2) at T = 298.15 K: ● – this work, ○ – Letcher and Nevines[9] ⊕ – Garriga et al.[10] □ – Iglesias et al.[12] Line – eq 11.

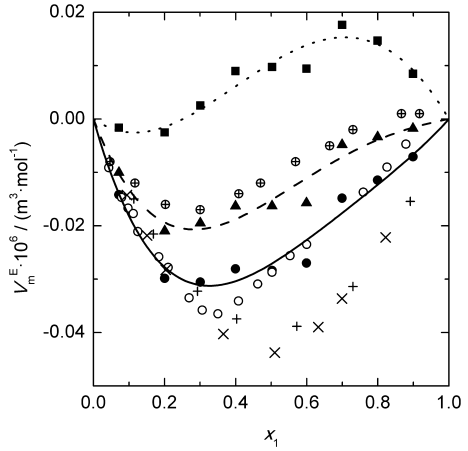

Figure 8. Excess molar volume of butan-2-one (1) + propan-1-ol (2). This work: ● – T = 298.15 K, ▲ – T = 303.15 K, ■ – T = 313.15 K; Letcher and Nevines:[9] ○ – T = 298.15 K; Garriga et al.:[10] ⊕ – T = 298.15 K; Subramanyam Reddy and Naidu:[27] + – T = 303.15 K, × – T = 313.15 K. Lines – eq 11.

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Table 9. Molar Excesses of Isentropic Compression and of Thermal Expansion of the Binary System Butanone-2 (1) + Ethanol (2) Calculated According to eq 8 from the Densities and Speeds of Sound Reported by Pereiro and Rodríguez[7]

x_1	T / K	$K^E_{S,m}\cdot10^{14}$ / $m^3\cdot mol^{-1}\cdot Pa^{-1}$	$E^E_{p,m}\cdot10^9$ / $m^3\cdot mol^{-1}\cdot K^{-1}$
0.0482	293.15	−0.0577	1.96
0.0482	298.15	−0.0405	0.33
0.0482	303.15	−0.0227	−1.33
0.1006	293.15	−0.1107	0.83
0.1006	298.15	−0.0691	0.64
0.1006	303.15	−0.0537	0.46
0.2005	293.15	−0.1683	3.17
0.2005	298.15	−0.1038	0.85
0.2005	303.15	−0.0758	−1.51
0.2998	293.15	−0.2053	0.27
0.2998	298.15	−0.1194	0.44
0.2998	303.15	−0.0900	0.64
0.3937	293.15	−0.2254	1.34
0.3937	298.15	−0.1237	0.34
0.3937	303.15	−0.0840	−0.66
0.4988	293.15	−0.2114	2.39
0.4988	298.15	−0.1109	0.18
0.4988	303.15	−0.0752	−2.06
0.5994	293.15	−0.2040	3.12
0.5994	298.15	−0.1124	1.24
0.5994	303.15	−0.0687	−0.65
0.7044	293.15	−0.1760	1.07
0.7044	298.15	−0.1014	1.45
0.7044	303.15	−0.0640	1.85
0.8017	293.15	−0.1482	4.68
0.8017	298.15	−0.0808	0.90
0.8017	303.15	−0.0526	−2.94
0.9017	293.15	−0.1014	0.09
0.9017	298.15	−0.0617	0.37
0.9017	303.15	−0.0268	0.67
0.9503	293.15	−0.0704	−2.72
0.9503	298.15	−0.0323	0.74
0.9503	303.15	−0.0053	4.26

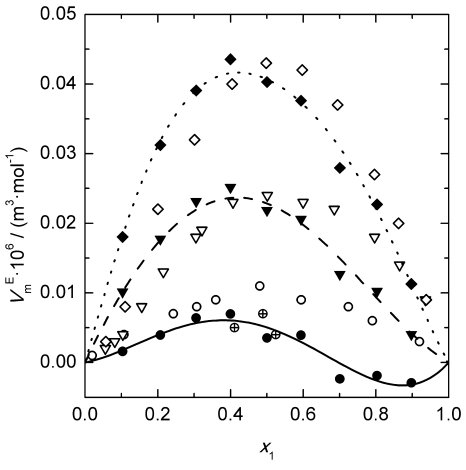

Figure 9. Excess molar volume of butan-2-one (1) + butan-1-ol (2). This work: • − T = 298.15 K, ▼ − T = 308.15 K, ◆ − T = 318.15 K; Iñarrea et al.:[11] ○ − T = 298.15 K; ⊕ − T = 308.15 K; Martínez et al.:[2] ∇ − T = 298.15 K; ◇ − T = 318.15 K. Lines − eq 11.

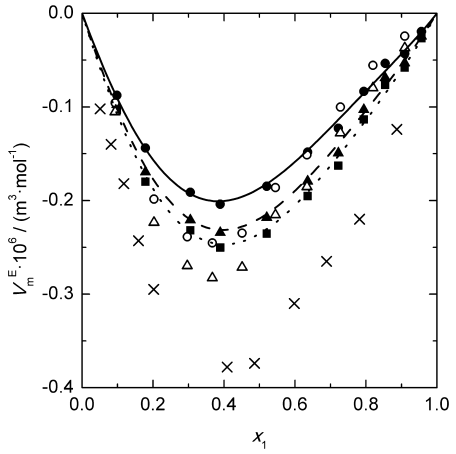

Figure 10. Excess molar volume of butan-2-one (1) + chloroform (2). This work: • − T = 293.15 K, ▲ − T = 303.15 K, ■ − T = 308.15 K; calculated from the densities reported by Clará, Gómez Marigliano and Sólimo:[16] ○ − T = 293.15 K; Δ − T = 308.15 K; Rama Varma, Kumaran, and Seetharaman:[28] × − T = 308.15 K. Lines − eq 11.

Molar isentropic compression of the ideal system is given by the following formula:

$$K^{id}_{S,m} = K^{id}_{T,m} - T(E^{id}_{p,m})^2/C^{id}_{p,m} \quad (10)$$

where $C^{id}_{p,m}$ is the molar isobaric heat capacity and $K^{id}_{T,m} \equiv -(\partial V_m/\partial p)_T$ is the molar isothermal compression. $C_{p,m}{}^{id}$ and $K_{T,m}{}^{id}$ satisfy eq 9. The molar isobaric heat capacities of the pure substances, $C^0_{p,i}$, were taken from the literature: butan-2-one,[21] methanol,[22] ethanol,[23] propan-1-ol,[24] butan-1-ol,[25] and chloroform.[26] Molar isothermal compressions of pure liquids were calculated from the isentropic ones, using the rearranged formula analogous to eq 10. The excesses are reported in Tables 2−5.

The following modified Redlich−Kister polynomials were used to approximate the excess functions:

$$\frac{Z^E_m}{x_1x_2} = \sum_{i=0}^{4}\sum_{j=0}^{2} a_{ij}(x_2 - x_1)^i\vartheta^j \quad (11)$$

where $Z = V\cdot10^6/(m^3\cdot mol^{-1})$ or $Z = K_S\cdot10^{15}/(m^3\cdot mol^{-1}\cdot Pa^{-1})$. The regression coefficients a_{ij}, calculated in the same way as the coefficients of eq 2, are reported in Tables 8 and 9. From the excess molar volume given by eq 11, the excess molar thermal expansion can be easily calculated: $E^E_m = (\partial V^E_m/\partial T)_p$.

Densities and speeds of sound for the system butan-2-one + ethanol have been measured by Pereiro and Rodriguez.[7] These authors reported also the excess volumes and the $V_m{}^E(x_1,T)$ polynomials but neither the excess expansions nor the excess isentropic compressions. Thus, we calculated the $E_{p,m}{}^E$ and $K_{S,m}{}^E$ for that system, applying the heat capacity of ethanol measured by Vega-Maza et al.,[23] and the results are reported in Table 9. The excess expansions proved to be very much scattered because of rather low precision of the densities, $1\cdot10^{-1}$ kg·m^{-3}, and of the narrow temperature range of the measurements, only of 10 K wide. Thus, the $E_{p,m}{}^E$ values only for T = 298.15 K, i.e. that in the middle of the temperature range, were taken into further consideration. The coefficients of eq 11 for the $K_{S,m}{}^E(x_1,T)$ of that system, calculated in the same way as for the other binaries, are given in Table 8.

Comparisons of the excess volumes obtained in this study with the literature ones are shown in Figures 7−10. The molar excesses of volume, thermal expansions, and isentropic compressions for

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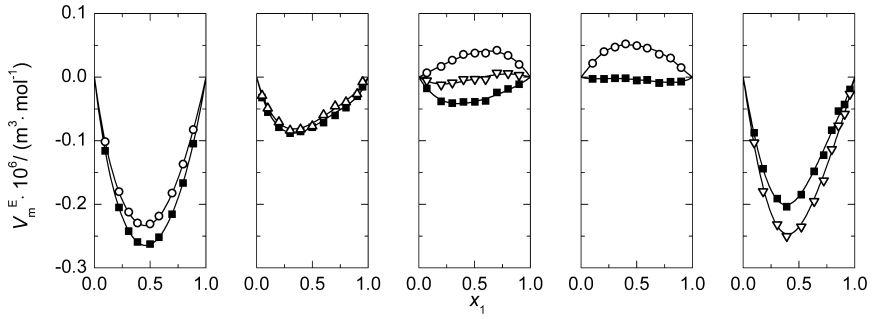

Figure 11. Excess molar volumes of binary systems butan-2-one (1) + cosolvent (2). Cosolvents from left to right: methanol, ethanol, propan-1-ol, butan-1-ol, chloroform. Data for methanol, propan-1-ol, butan-1-ol, and chloroform − this work, ethanol − Pereiro and Rodríguez.[7] Points − experimental results: ■ − T = 293.15 K, Δ − T = 303.15 K, ∇ − T = 308.15 K, ○ − T = 323.15 K; lines − eq 11.

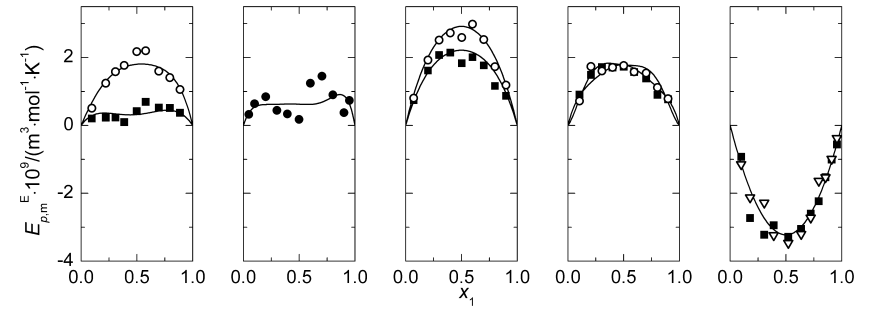

Figure 12. Excess molar expansions of binary systems butan-2-one (1) + cosolvent (2). Cosolvents from left to right: methanol, ethanol, propan-1-ol, butan-1-ol, chloroform. Data for methanol, propan-1-ol, butan-1-ol, and chloroform − this work, ethanol − Pereiro and Rodríguez.[7] Points − experimental results: ■ − T = 293.15 K, ● − T = 298.15 K, ∇ − T = 308.15 K, ○ − T = 323.15 K; lines − temperature derivative of V^E given by eq 11.

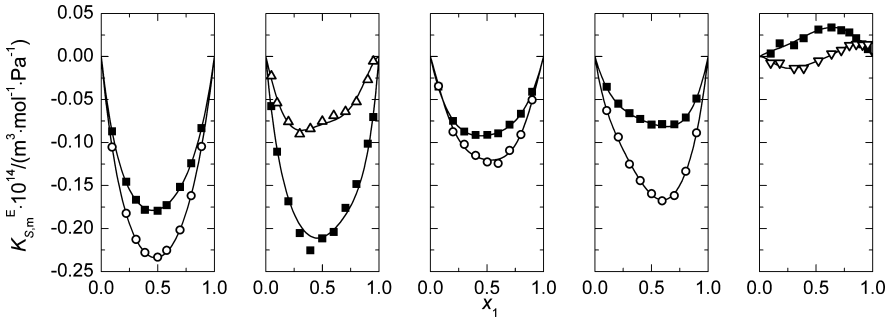

Figure 13. Excess molar isentropic compression of binary systems butan-2-one (1) + cosolvent (2). Cosolvents from left to right: methanol, ethanol, propan-1-ol, butan-1-ol, chloroform. Data for methanol, propan-1-ol, butan-1-ol, and chloroform−this work, ethanol − Pereiro and Rodríguez.[7] Points−experimental results: ■ − T = 293.15 K, Δ − T = 303.15 K, ∇ − T = 308.15 K, ○ − T = 323.15 K; lines − eq 11.

all five binary systems are plotted in Figures 11, 12, and 13, respectively.

■ DISCUSSION AND CONCLUSIONS

All the investigated mixtures are thermodynamically nonideal. The excess volumes are negative for the mixtures with methanol and ethanol and S-shaped for those with propan-1-ol and butan-1-ol (Figures 8, 9, 11). The change of sign of the V^E on elongation of the hydrocarbon chain in the alcohol molecule probably results mainly from the changes in the spatial arrangement of the molecules in the mixtures in comparison with that in the pure liquids. Small molecules of methanol partially fill in the gaps between the molecules of butan-2-one. Those of propan-1-ol and butan-1-ol, being of similar size to the butan-2-one ones, are incapable of such behavior. That makes the negative V^E smaller, or even leads to positive V^E values for higher temperatures. The hydrogen bond energy seems to play a less important role, especially in the mixtures containing the alcohols with long-chain molecules, as the difference in the proton affinity between the C═O group in butan-2-one and the OH one in the alcohols decreases with the elongation of the chain length. The proton affinities are 827.3 kJ·mol^{-1} for butan-2-one and (754.3, 776.4, 786.5 and 789.2) kJ·mol^{-1} for methanol, ethanol, propan-1-ol and butan-1-ol, respectively.[29] Slightly higher values for methanol and ethanol were obtained by quantum chemical calculations: (773.6 and 796.2) kJ·mol^{-1} by MP2/aVDZ++ and (776.6 and 802.9) kJ·mol^{-1} by B3LYP/aVDZ++.[30] Thus, the O−H···O═C bonds between the unlike molecules arise, that are slightly stronger than those in pure alcohols. Nevertheless, the cross-association effect on enthalpy is too small to overcome its decrease due to the disintegration of the alcohol self-associates.[31] That is manifested in positive excess enthalpies, with maximum values of ca. (0.7, 1.1, 1.3 and 1.4) kJ·mol^{-1} for methanol,[3,32] ethanol,[3,32] propan-1-ol[3,33] and butan-1-ol + butan-2-one,[8] respectively.

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An increase of the temperature causes dissociation of the hydrogen-bonded associates that leads to positive changes of the V^E, i.e. to positive values of the excess thermal expansions of the mixtures with alcohols, as it is illustrated in Figure 12. Since

$$E_p^E = (\partial V^E/\partial T)_p = -(\partial S^E/\partial p)_T \quad (12)$$

the $E_p^E > 0$ evidence that the excess entropy decreases with increasing pressure, i.e. that pressure makes the systems more ordered.

The excess molar isentropic compression is negative for the alcoholic mixtures (Figure 13). The opposite signs of the excesses of isentropic compression and of thermal expansion reflect the counteracting effects of pressure and temperature on the excess volume. The negative K_S^E values increase with increasing temperature for the mixtures with methanol, propan-1-ol, and butan-1-ol. The trend seems to be opposite to that with ethanol. However, rather low precision of the data for butan-2-one + ethanol[7] makes a definite explanation of this discrepancy impossible. It is evident, however, that the O−H···O═C bonds make the system stiffer and less compressible in comparison with the respective ideal mixture.

The excess volume of butan-2-one + chloroform is negative, which is similar to the V^E of the mixtures containing methanol and ethanol (Figure 11). The reasons for that, however, seem to be different. Contrary to the two pure alcohols, chloroform does not self-associate. In the binary mixture with butan-2-one, the 1:1 and 1:2 butan-2-one−chloroform cross-associates occur due to the C−H···O hydrogen bonds, as it was confirmed by the FT-IR Raman spectra.[34] Differences in the energies between the monomers and the complexes are (17 to 18) kJ·mol^{-1} for the dimer and (25 to 26) kJ·mol^{-1} for the trimer, calculated with the B3LYP functional and different basis sets.[34] It should be noted, however, that the theoretically calculated energies are usually higher than those obtained from thermodynamic data or from infrared spectroscopy, as it was shown for several alcohol−alkanone systems.[32] Nevertheless, the formation of the butan-2-one−chloroform cross-associates makes the mixing highly exothermic, with the maximum negative excess enthalpy of −1.4 kJ·mol^{-1} for T = 303 K.[34]

The negative excess thermal expansion of butan-2-one + chloroform (Figure 12) points to an increase of the excess entropy on increasing pressure (eq 12). Although elevated pressures favor the formation of the hydrogen bonds, the effect is evidently too weak to compensate for the increase of the S^E caused by the simultaneous decrease of the free volume. Thus, if the intermolecular distances are shorter (i.e., if the free volume is smaller), then the difference in shapes of the two types of molecules stronger influences the molecular order in the mixture. The excess compression of butan-2-one + chloroform is small in comparison with those of the systems containing alcohols (Figure 13). Thus, the formation of the C−H···O bonds influences the compressibility rather weakly. It should be noted that the 1:1 and 1:2 complexes of butan-2-one with chloroform are incapable of further aggregation because of the lack of free proton-donating and proton-accepting groups in the complex. That makes this system considerably different from those with alcohols, whose molecules are able to form larger clusters.

AUTHOR INFORMATION

Corresponding Author

*E-mail: w.marczak@imp.sosnowiec.pl.

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