Volumetric Properties of the Binary Methanol + Chloroform and Ternary Methanol + Chloroform + Benzene Mixtures at (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K

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Densities ρ of the ternary system of methanol + chloroform + benzene and binary mixture of methanol + chloroform have been measured at six temperatures (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K and atmospheric pressure with an Anton Paar DMA 5000 digital vibrating tube densimeter. Excess molar volumes V^E were calculated from the densities data and correlated by the Redlich−Kister (for binary data) and Nagata−Tamura (for ternary data) equations.

Introduction

This paper is continuation of our study[1−4] of the volumetric properties of binaries and multicomponent mixtures containing different types of organic solvents widely used in various industries. As has already been mentioned,[3,4] thermodynamic investigation of alcohols, chloroform, and aromatics alone or in mixtures is of great interest due to the complex molecular interactions present in these mixtures and their diverse industry application (e.g., extraction of the penicillin and other antibiotics in pharmaceutical industry; for pesticides, fats, oils, rubber, alkaloids, waxes, etc; chloroform with alcohols or benzene is widely used as an eluting system in medical purposes, in radiopharmacy, in chemical reactions, etc.). Also, chloroform and benzene are usually contained in wastewater from different industries as pollutants having cancerous tendencies.

In the present work, we have measured densities ρ for the ternary system of methanol + chloroform + benzene, and the binary system of methanol + chloroform at temperatures of (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K and atmospheric pressure. The related property, excess molar volume V^E, was calculated from the measured data. The V^E of binary data were fitted using the Redlich−Kister[5] equation, while the Nagata and Tamura[6] equation was used for the ternary data.

For the binary mixture methanol + chloroform, the ρ and V^E literature data cover only temperatures 298.15 K[7,8] and 303.15 K.[9] In the currently published articles, there are no values of V^E for the other temperatures studied here. Also, for the investigated ternary system, literature data are not available.

Experimental Section

Chemicals. Methanol (Merck) was supplied with 99.8 % purity (p.a.). Chloroform (stabilized with amylene) was supplied by Riedel-de Haën with a purity of 99.8 %, while benzene was supplied by Aldrich with a purity of 99.9 % (HPLC). Table 1 lists the measured densities of the methanol, chloroform, and benzene, which agreed to within ± 0.08 kg m^{-3} with the most of corresponding literature values.[2,10−12] Since the agreement is very good, all the compounds were used without further purification.

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Table 1. Densities ρ of the Pure Components at 298.15 K and Atmospheric Pressure

	$\rho \times 10^{-3}$/(kg·m^{-3})	
component	exptl	lit
methanol	0.786694	0.78637[a], 0.78664[b]
chloroform	1.479148	1.47970[a], 1.47919[c]
benzene	0.873582	0.87360[a], 0.87362[d], 0.87364[b]

[a] Ref 10. [b] Ref 11. [c] Ref 12. [d] Ref 2.

Measurements. Densities ρ of the ternary methanol + chloroform + benzene system, the binary methanol + chloroform system, and corresponding pure substances were measured by means of an Anton Paar DMA 5000 digital vibrating U-tube densimeter (with automatic viscosity correction) having a stated accuracy of ± 5 × 10^{-3} kg·m^{-3}. The temperature in the cell was regulated to ± 0.001 K with a built-in solid-state thermostat. To minimize the errors in composition, all mixtures were prepared by mass using the cell and the procedure described previously.[13,14] Presently, a Mettler AG 204 balance with a precision of 1 × 10^{-4} g was used. The uncertainty of the mole fraction calculation was less than ± 1 × 10^{-4}. All molar quantities were based on the IUPAC relative atomic mass table. The experimental uncertainty in the density is about ± 1 × 10^{-2} kg·m^{-3}, while the average uncertainty in excess molar volume is estimated to be ± 3 × 10^{-9} m^{-3}·mol^{-1}.

Results and Discussion

The excess molar volumes V^E were calculated from

$$V^E = \sum_{i=1}^{n} x_i M_i [(1/\rho) - (1/\rho_i)] \quad (1)$$

where n is the number of components; x_i is the mole fraction of component i in the mixture; M_i is its molecular weight; and ρ and ρ_i are the measured densities of the mixture and the pure component i, respectively.

Tables 2 and 3 list the measured densities ρ and the corresponding values of V^E for the binary methanol + chloroform system and the ternary methanol + chloroform + benzene

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Table 2. Densities ρ and Excess Molar Volumes V^E for Methanol (1) + Chloroform (2) from T = (288.15 to 313.15) K and Atmospheric Pressure

x_1	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}
Methanol (1) + Chloroform (2)											
T = 288.15 K											
0.0000	1.498077	0.0000	0.2444	1.401121	−0.0808	0.6022	1.197323	−0.1590	0.9100	0.911539	−0.0236
0.0298	1.487346	0.0004	0.2956	1.377441	−0.1050	0.6352	1.172938	−0.1551	0.9300	0.887399	−0.0124
0.0492	1.480267	−0.0036	0.3383	1.356507	−0.1218	0.6999	1.121290	−0.1334	0.9542	0.857083	−0.0032
0.0724	1.471759	−0.0159	0.3980	1.325255	−0.1399	0.7500	1.077545	−0.1092	1.0000	0.796093	0.0000
0.0942	1.463439	−0.0204	0.4393	1.302229	−0.1519	0.7996	1.030616	−0.0796			
0.1282	1.450192	−0.0332	0.4983	1.267100	−0.1670	0.8193	1.011238	−0.0829			
0.1586	1.437963	−0.0462	0.5505	1.233392	−0.1683	0.8534	0.975440	−0.0556			
T = 293.15 K											
0.0000	1.488638	0.0000	0.2444	1.392244	−0.0748	0.6022	1.190011	−0.1610	0.9100	0.906188	−0.0278
0.0298	1.477931	0.0032	0.2956	1.368733	−0.0993	0.6352	1.165776	−0.1563	0.9300	0.882191	−0.0159
0.0492	1.470881	0.0003	0.3383	1.347953	−0.1167	0.6999	1.114520	−0.1365	0.9542	0.852051	−0.0057
0.0724	1.462414	−0.0110	0.3980	1.316934	−0.1357	0.7500	1.071098	−0.1136	1.0000	0.791400	0.0000
0.0942	1.454141	−0.0149	0.4393	1.294082	−0.1484	0.7996	1.024500	−0.0847			
0.1282	1.440980	−0.0274	0.4983	1.259218	−0.1646	0.8193	1.005113	−0.0815			
0.1586	1.428829	−0.0401	0.5505	1.225765	−0.1672	0.8534	0.969692	−0.0609			
T = 298.15 K											
0.0000	1.479148	0.0000	0.2444	1.383302	−0.0676	0.6022	1.182624	−0.1610	0.9100	0.900813	−0.0317
0.0298	1.468465	0.0062	0.2956	1.359967	−0.0927	0.6352	1.158565	−0.1567	0.9300	0.876963	−0.0193
0.0492	1.461441	0.0046	0.3383	1.339334	−0.1102	0.6999	1.107707	−0.1390	0.9542	0.847000	−0.0082
0.0724	1.453013	−0.0056	0.3980	1.308550	−0.1301	0.7500	1.064609	−0.1173	1.0000	0.786694	0.0000
0.0942	1.444789	−0.0090	0.4393	1.285874	−0.1437	0.7996	1.018344	−0.0891			
0.1282	1.431705	−0.0207	0.4983	1.251280	−0.1613	0.8193	0.998988	−0.0812			
0.1586	1.419634	−0.0330	0.5505	1.218088	−0.1652	0.8534	0.963915	−0.0658			
T = 303.15 K											
0.0000	1.469612	0.0000	0.2444	1.374295	−0.0590	0.6022	1.175169	−0.1594	0.9100	0.895410	−0.0357
0.0298	1.458953	0.0092	0.2956	1.351137	−0.0848	0.6352	1.151299	−0.1561	0.9300	0.871710	−0.0228
0.0492	1.451950	0.0093	0.3383	1.330656	−0.1026	0.6999	1.100844	−0.1407	0.9542	0.841927	−0.0107
0.0724	1.443554	0.0006	0.3980	1.300105	−0.1233	0.7500	1.058072	−0.1202	1.0000	0.781966	0.0000
0.0942	1.435375	−0.0020	0.4393	1.277602	−0.1376	0.7996	1.012148	−0.0932			
0.1282	1.422367	−0.0127	0.4983	1.243281	−0.1567	0.8193	0.992860	−0.0821			
0.1586	1.410374	−0.0247	0.5505	1.210350	−0.1619	0.8534	0.958100	−0.0704			
T = 308.15 K											
0.0000	1.460025	0.0000	0.2444	1.365219	−0.0490	0.6022	1.167650	−0.1565	0.9100	0.889975	−0.0396
0.0298	1.449385	0.0126	0.2956	1.342240	−0.0756	0.6352	1.143978	−0.1546	0.9300	0.866422	−0.0261
0.0492	1.442400	0.0146	0.3383	1.321902	−0.0932	0.6999	1.093926	−0.1415	0.9542	0.836829	−0.0135
0.0724	1.434035	0.0076	0.3980	1.291589	−0.1150	0.7500	1.051484	−0.1225	1.0000	0.777213	0.0000
0.0942	1.425891	0.0064	0.4393	1.269262	−0.1301	0.7996	1.005907	−0.0967			
0.1282	1.412964	−0.0037	0.4983	1.235216	−0.1508	0.8193	0.986761	−0.0861			
0.1586	1.401043	−0.0149	0.5505	1.202554	−0.1577	0.8534	0.952240	−0.0744			
T = 313.15 K											
0.0000	1.450413	0.0000	0.2444	1.356097	−0.0377	0.6022	1.160084	−0.1524	0.9100	0.884513	−0.0431
0.0298	1.439804	0.0155	0.2956	1.333290	−0.0646	0.6352	1.136625	−0.1526	0.9300	0.861110	−0.0291
0.0492	1.432835	0.0195	0.3383	1.313094	−0.0821	0.6999	1.086962	−0.1411	0.9542	0.831705	−0.0159
0.0724	1.424490	0.0148	0.3980	1.283024	−0.1052	0.7500	1.044851	−0.1236	1.0000	0.772443	0.0000
0.0942	1.416399	0.0139	0.4393	1.260885	−0.1218	0.7996	0.999622	−0.0992			
0.1282	1.403524	0.0062	0.4983	1.227126	−0.1446	0.8193	0.980633	−0.0897			
0.1586	1.391678	−0.0043	0.5505	1.194712	−0.1522	0.8534	0.946342	−0.0776			

system. Experimental results for the other two binary systems methanol + benzene and chloroform + benzene have been presented in our previous papers.[3,4]

Comparison of our experimental results of V^E at (298.15 and 303.15) K with data reported previously for the system methanol + chloroform[7−9] shows that discrepancies for the investigated binary system, at $x_1 = 0.5$ are ($0.020 \cdot 10^{-6}$, $0.006 \cdot 10^{-6}$, and $0.009 \cdot 10^{-6}$) m^3·mol^{-1}, respectively.

Data for the binary mixtures were correlated with the Redlich−Kister[5] (RK) polynomial:

$$V_{ij}^E/10^{-6}\ \mathrm{m^3 \cdot mol^{-1}} = x_i x_j \sum_{p=0}^{k} A_p (2x_i - 1)^p \qquad (2)$$

where A_p denotes the adjustable parameters, and $k + 1$ is the number of adjustable parameters determined by means of the *F*-test. Adjustable parameters of the fits at each temperature separately and the corresponding root-mean-square deviations (rmsd) defined by

$$\sigma = \left(\sum_{i=1}^{m} (V_{\mathrm{exp},i}^E - V_{\mathrm{cal},i}^E)^2/m\right)^{1/2} \qquad (3)$$

are given in Table 4. In eq 3, m is the number of experimental data points.

The V^E data for ternary system were correlated by the Nagata and Tamura[6] model:

$$V_{123}^E/10^{-6}\ \mathrm{m^3 \cdot mol^{-1}} = V_{12}^E + V_{13}^E + V_{23}^E + x_1 x_2 x_3 RT(B_0 - B_1 x_1 - B_2 x_2 - B_3 x_1^2 - B_4 x_2^2 - B_5 x_1 x_2 - B_6 x_1^3 - B_7 x_2^3 - B_8 x_1^2 x_2) \qquad (4)$$

Table 3. Densities ρ and Excess Molar Volumes V^E for Methanol (1) + Chloroform (2) + Benzene (3) from T = (288.15 to 313.15) K and Atmospheric Pressure

x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}
						T = 288.15 K									
0.0192	0.8016	1.368917	0.1023	0.0976	0.5009	1.186422	0.1621	0.0598	0.9015	1.449115	0.0101	0.3992	0.5007	1.241361	−0.0552
0.0296	0.6985	1.303088	0.1428	0.1199	0.3988	1.123082	0.1648	0.1195	0.7988	1.394494	0.0270	0.4777	0.4014	1.175042	−0.0496
0.0404	0.6000	1.241336	0.1604	0.1412	0.2988	1.060835	0.1600	0.1827	0.6964	1.338345	0.0236	0.4885	0.4252	1.197407	−0.0748
0.0494	0.5004	1.179370	0.1782	0.1601	0.2002	0.999417	0.1374	0.2388	0.6020	1.282813	0.0315	0.5604	0.3006	1.101164	−0.0329
0.0496	0.5011	1.179783	0.1797	0.1784	0.1022	0.938572	0.0867	0.3005	0.4996	1.219550	0.0383	0.6400	0.2005	1.019575	−0.0186
0.0566	0.4023	1.118783	0.1915	0.0424	0.8986	1.441490	0.0289	0.3580	0.4009	1.154649	0.0382	0.7206	0.1002	0.928648	−0.0008
0.0666	0.3002	1.057071	0.1738	0.0791	0.7995	1.383499	0.0549	0.3669	0.4111	1.163870	0.0295	0.1829	0.7986	1.413916	−0.0373
0.0777	0.2015	0.998153	0.1431	0.1192	0.7014	1.325720	0.0729	0.4196	0.3003	1.084812	0.0474	0.2667	0.7034	1.367586	−0.0705
0.0881	0.1008	0.938735	0.0886	0.1578	0.5998	1.263561	0.0937	0.4800	0.2004	1.011071	0.0422	0.3586	0.6020	1.313627	−0.0876
0.0968	0.1002	0.938272	0.0893	0.1984	0.5012	1.202097	0.1207	0.5408	0.0998	0.932271	0.0120	0.4515	0.4993	1.252640	−0.1050
0.0233	0.8952	1.433328	0.0478	0.2433	0.3981	1.136850	0.1066	0.0789	0.9028	1.456092	−0.0032	0.5396	0.4011	1.186718	−0.0974
0.0383	0.8010	1.373387	0.0946	0.2804	0.3017	1.073145	0.1085	0.1585	0.7993	1.406704	−0.0161	0.6294	0.3008	1.110632	−0.0705
0.0603	0.6995	1.310564	0.1207	0.3190	0.2029	1.006366	0.0938	0.2381	0.7020	1.357857	−0.0332	0.7198	0.1995	1.023657	−0.0429
0.0785	0.5994	1.247800	0.1495	0.3594	0.1007	0.935475	0.0597	0.3208	0.6004	1.302125	−0.0485	0.8096	0.1004	0.926523	−0.0142
						T = 293.15 K									
0.0192	0.8016	1.360432	0.0993	0.0976	0.5009	1.179190	0.1581	0.0598	0.9015	1.439960	0.0135	0.3992	0.5007	1.233687	−0.0543
0.0296	0.6985	1.295071	0.1387	0.1199	0.3988	1.116271	0.1607	0.1195	0.7988	1.385725	0.0302	0.4777	0.4014	1.167855	−0.0506
0.0404	0.6000	1.233748	0.1555	0.1412	0.2988	1.054425	0.1564	0.1827	0.6964	1.329982	0.0258	0.4885	0.4252	1.190056	−0.0750
0.0494	0.5004	1.172209	0.1723	0.1601	0.2002	0.993390	0.1350	0.2388	0.6020	1.274854	0.0326	0.5604	0.3006	1.094506	−0.0356
0.0496	0.5011	1.172618	0.1739	0.1784	0.1022	0.932910	0.0865	0.3005	0.4996	1.212049	0.0378	0.6400	0.2005	1.013478	−0.0224
0.0566	0.4023	1.112016	0.1859	0.0424	0.8986	1.432416	0.0307	0.3580	0.4009	1.147608	0.0364	0.7206	0.1002	0.923144	−0.0045
0.0666	0.3002	1.050695	0.1691	0.0791	0.7995	1.374839	0.0563	0.3669	0.4111	1.156762	0.0281	0.1829	0.7986	1.404959	−0.0316
0.0777	0.2015	0.992137	0.1401	0.1192	0.7014	1.317477	0.0733	0.4196	0.3003	1.078250	0.0448	0.2667	0.7034	1.358966	−0.0657
0.0881	0.1008	0.933070	0.0881	0.1578	0.5998	1.255760	0.0931	0.4800	0.2004	1.004999	0.0393	0.3586	0.6020	1.305405	−0.0841
0.0968	0.1002	0.932608	0.0891	0.1984	0.5012	1.194908	0.1079	0.5408	0.0998	0.926700	0.0096	0.4515	0.4993	1.244871	−0.1032
0.0233	0.8952	1.424347	0.0476	0.2433	0.3981	1.129934	0.1040	0.0789	0.9028	1.446863	0.0014	0.5396	0.4011	1.179446	−0.0980
0.0383	0.8010	1.364839	0.0936	0.2804	0.3017	1.066646	0.1062	0.1585	0.7993	1.397817	−0.0113	0.6294	0.3008	1.103923	−0.0734
0.0603	0.6995	1.302463	0.1188	0.3190	0.2029	1.000300	0.0917	0.2381	0.7020	1.349321	−0.0290	0.7198	0.1995	1.017556	−0.0472
0.0785	0.5994	1.240145	0.1464	0.3594	0.1007	0.929849	0.0589	0.3208	0.6004	1.293999	−0.0457	0.8096	0.1004	0.921055	−0.0183
						T = 298.15 K									
0.0192	0.8016	1.351904	0.0964	0.0976	0.5009	1.171916	0.1551	0.0598	0.9015	1.430754	0.0171	0.3992	0.5007	1.225954	−0.0520
0.0296	0.6985	1.287013	0.1349	0.1199	0.3988	1.109421	0.1578	0.1195	0.7988	1.376895	0.0345	0.4777	0.4014	1.160615	−0.0503
0.0404	0.6000	1.226124	0.1508	0.1412	0.2988	1.047980	0.1540	0.1827	0.6964	1.321560	0.0293	0.4885	0.4252	1.182656	−0.0743
0.0494	0.5004	1.165010	0.1671	0.1601	0.2002	0.987329	0.1341	0.2388	0.6020	1.266844	0.0346	0.5604	0.3006	1.087805	−0.0373
0.0496	0.5011	1.165413	0.1690	0.1784	0.1022	0.927220	0.0877	0.3005	0.4996	1.204493	0.0388	0.6400	0.2005	1.007345	−0.0253
0.0566	0.4023	1.105219	0.1809	0.0424	0.8986	1.423296	0.0326	0.3580	0.4009	1.140514	0.0362	0.7206	0.1002	0.917607	−0.0073
0.0666	0.3002	1.044290	0.1651	0.0791	0.7995	1.366128	0.0583	0.3669	0.4111	1.149608	0.0277	0.1829	0.7986	1.395942	−0.0249
0.0777	0.2015	0.986093	0.1381	0.1192	0.7014	1.309182	0.0746	0.4196	0.3003	1.071644	0.0435	0.2667	0.7034	1.350284	−0.0596
0.0881	0.1008	0.927383	0.0887	0.1578	0.5998	1.247911	0.0935	0.4800	0.2004	0.998890	0.0375	0.3586	0.6020	1.297124	−0.0793
0.0968	0.1002	0.926922	0.0898	0.1984	0.5012	1.187594	0.1010	0.5408	0.0998	0.921097	0.0084	0.4515	0.4993	1.237051	−0.1005
0.0233	0.8952	1.415320	0.0476	0.2433	0.3981	1.122976	0.1025	0.0789	0.9028	1.437581	0.0065	0.5396	0.4011	1.172121	−0.0974
0.0383	0.8010	1.356246	0.0929	0.2804	0.3017	1.060115	0.1046	0.1585	0.7993	1.388870	−0.0055	0.6294	0.3008	1.097168	−0.0753
0.0603	0.6995	1.294318	0.1173	0.3190	0.2029	0.994202	0.0907	0.2381	0.7020	1.340724	−0.0237	0.7198	0.1995	1.011418	−0.0508
0.0785	0.5994	1.232445	0.1440	0.3594	0.1007	0.924193	0.0594	0.3208	0.6004	1.285815	−0.0417	0.8096	0.1004	0.915556	−0.0217
						T = 303.15 K									
0.0192	0.8016	1.343332	0.0939	0.0976	0.5009	1.164595	0.1534	0.0598	0.9015	1.421494	0.0215	0.3992	0.5007	1.218167	−0.0485
0.0296	0.6985	1.278914	0.1315	0.1199	0.3988	1.102528	0.1561	0.1195	0.7988	1.368014	0.0395	0.4777	0.4014	1.153320	−0.0487
0.0404	0.6000	1.218458	0.1468	0.1412	0.2988	1.041495	0.1530	0.1827	0.6964	1.313081	0.0340	0.4885	0.4252	1.175202	−0.0725
0.0494	0.5004	1.157779	0.1622	0.1601	0.2002	0.981237	0.1342	0.2388	0.6020	1.258783	0.0377	0.5604	0.3006	1.081054	−0.0378
0.0496	0.5011	1.158174	0.1644	0.1784	0.1022	0.921500	0.0901	0.3005	0.4996	1.196890	0.0407	0.6400	0.2005	1.001169	−0.0273
0.0566	0.4023	1.098387	0.1765	0.0424	0.8986	1.414124	0.0351	0.3580	0.4009	1.133371	0.0371	0.7206	0.1002	0.912041	−0.0097
0.0666	0.3002	1.037855	0.1618	0.0791	0.7995	1.357363	0.0612	0.3669	0.4111	1.142403	0.0287	0.1829	0.7986	1.386863	−0.0170
0.0777	0.2015	0.980022	0.1369	0.1192	0.7014	1.300835	0.0769	0.4196	0.3003	1.064992	0.0434	0.2667	0.7034	1.341539	−0.0522
0.0881	0.1008	0.921668	0.0903	0.1578	0.5998	1.240011	0.0950	0.4800	0.2004	0.992742	0.0367	0.3586	0.6020	1.288781	−0.0733
0.0968	0.1002	0.921208	0.0917	0.1984	0.5012	1.180148	0.1005	0.5408	0.0998	0.915457	0.0084	0.4515	0.4993	1.229168	−0.0963
0.0233	0.8952	1.406243	0.0479	0.2433	0.3981	1.115975	0.1021	0.0789	0.9028	1.428239	0.0125	0.5396	0.4011	1.164742	−0.0957
0.0383	0.8010	1.347606	0.0926	0.2804	0.3017	1.053538	0.1046	0.1585	0.7993	1.379859	0.0016	0.6294	0.3008	1.090362	−0.0763
0.0603	0.6995	1.286125	0.1167	0.3190	0.2029	0.988064	0.0911	0.2381	0.7020	1.332068	−0.0171	0.7198	0.1995	1.005235	−0.0536
0.0785	0.5994	1.224698	0.1427	0.3594	0.1007	0.918504	0.0612	0.3208	0.6004	1.277572	−0.0364	0.8096	0.1004	0.910028	−0.0249
						T = 308.15 K									
0.0192	0.8016	1.334715	0.0915	0.0976	0.5009	1.157230	0.1526	0.0598	0.9015	1.412178	0.0263	0.3992	0.5007	1.210308	−0.0431
0.0296	0.6985	1.270769	0.1286	0.1199	0.3988	1.095596	0.1553	0.1195	0.7988	1.359075	0.0454	0.4777	0.4014	1.145962	−0.0455
0.0404	0.6000	1.210744	0.1438	0.1412	0.2988	1.034972	0.1531	0.1827	0.6964	1.304546	0.0396	0.4885	0.4252	1.167684	−0.0692
0.0494	0.5004	1.150508	0.1578	0.1601	0.2002	0.975112	0.1354	0.2388	0.6020	1.250660	0.0422	0.5604	0.3006	1.074257	−0.0376
0.0496	0.5011	1.150897	0.1603	0.1784	0.1022	0.915752	0.0935	0.3005	0.4996	1.189223	0.0444	0.6400	0.2005	0.994946	−0.0283
0.0566	0.4023	1.091516	0.1731	0.0424	0.8986	1.404899	0.0380	0.3580	0.4009	1.126172	0.0396	0.7206	0.1002	0.906438	−0.0115
0.0666	0.3002	1.031382	0.1597	0.0791	0.7995	1.348551	0.0644	0.3669	0.4111	1.135143	0.0310	0.1829	0.7986	1.377722	−0.0081
0.0777	0.2015	0.973921	0.1365	0.1192	0.7014	1.292435	0.0801	0.4196	0.3003	1.058283	0.0452	0.2667	0.7034	1.332731	−0.0437
0.0881	0.1008	0.915926	0.0930	0.1578	0.5998	1.232057	0.0977	0.4800	0.2004	0.986547	0.0374	0.3586	0.6020	1.280368	−0.0656
0.0968	0.1002	0.915468	0.0945	0.1984	0.5012	1.172629	0.1027	0.5408	0.0998	0.909781	0.0093	0.4515	0.4993	1.221221	−0.0908
0.0233	0.8952	1.397116	0.0485	0.2433	0.3981	1.108932	0.1026	0.0789	0.9028	1.418836	0.0194	0.5396	0.4011	1.157303	−0.0927
0.0383	0.8010	1.338912	0.0931	0.2804	0.3017	1.046916	0.1060	0.1585	0.7993	1.370777	0.0104	0.6294	0.3008	1.083500	−0.0761
0.0603	0.6995	1.277880	0.1169	0.3190	0.2029	0.981882	0.0931	0.2381	0.7020	1.323346	−0.0091	0.7198	0.1995	0.999004	−0.0555
0.0785	0.5994	1.216905	0.1421	0.3594	0.1007	0.912774	0.0646	0.3208	0.6004	1.269264	−0.0296	0.8096	0.1004	0.904459	−0.0275

Table 3. (Continued)

x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \times 10^{-3}$ / kg·m^{-3}	$V^E \times 10^6$ / m^3·mol^{-1}
$T = 313.15$ K															
0.0192	0.8016	1.326078	0.0889	0.0976	0.5009	1.149848	0.1517	0.0598	0.9015	1.402828	0.0319	0.3992	0.5007	1.202418	−0.0370
0.0296	0.6985	1.262613	0.1250	0.1199	0.3988	1.088634	0.1554	0.1195	0.7988	1.350105	0.0519	0.4777	0.4014	1.138570	−0.0415
0.0404	0.6000	1.203021	0.1399	0.1412	0.2988	1.028420	0.1543	0.1827	0.6964	1.295978	0.0461	0.4885	0.4252	1.160113	−0.0641
0.0494	0.5004	1.143218	0.1535	0.1601	0.2002	0.968970	0.1368	0.2388	0.6020	1.242491	0.0482	0.5604	0.3006	1.067434	−0.0371
0.0496	0.5011	1.143608	0.1558	0.1784	0.1022	0.909981	0.0978	0.3005	0.4996	1.181496	0.0506	0.6400	0.2005	0.988679	−0.0279
0.0566	0.4023	1.084631	0.1694	0.0424	0.8986	1.395642	0.0415	0.3580	0.4009	1.118952	0.0423	0.7206	0.1002	0.900799	−0.0121
0.0666	0.3002	1.024884	0.1584	0.0791	0.7995	1.339711	0.0680	0.3669	0.4111	1.127846	0.0345	0.1829	0.7986	1.368540	0.0020
0.0777	0.2015	0.967811	0.1357	0.1192	0.7014	1.284020	0.0829	0.4196	0.3003	1.051537	0.0482	0.2667	0.7034	1.323869	−0.0332
0.0881	0.1008	0.910174	0.0955	0.1578	0.5998	1.224085	0.1004	0.4800	0.2004	0.980321	0.0391	0.3586	0.6020	1.271909	−0.0564
0.0968	0.1002	0.909705	0.0984	0.1984	0.5012	1.165089	0.1050	0.5408	0.0998	0.904074	0.0114	0.4515	0.4993	1.213238	−0.0844
0.0233	0.8952	1.387968	0.0490	0.2433	0.3981	1.101899	0.1011	0.0789	0.9028	1.409405	0.0267	0.5396	0.4011	1.149821	−0.0886
0.0383	0.8010	1.330201	0.0933	0.2804	0.3017	1.040265	0.1082	0.1585	0.7993	1.361636	0.0213	0.6294	0.3008	1.076591	−0.0745
0.0603	0.6995	1.269579	0.1194	0.3190	0.2029	0.975677	0.0957	0.2381	0.7020	1.314581	0.0001	0.7198	0.1995	0.992738	−0.0566
0.0785	0.5994	1.209086	0.1420	0.3594	0.1007	0.907022	0.0689	0.3208	0.6004	1.260916	−0.0217	0.8096	0.1004	0.898864	−0.0297

Table 4. Parameters $A_p/10^{-6}$ m^3·mol^{-1} of Equation 2 and the Corresponding rmsd $\sigma/10^{-6}$ m^3·mol^{-1} for Binary Mixtures

T/K	A_0	A_1	A_2	A_3	σ
Methanol (1) + Chloroform (2)					
288.15	−0.6598	−0.2092	0.5787	0.2536	0.0034
293.15	−0.6530	−0.2536	0.5845	0.2242	0.0028
298.15	−0.6413	−0.3003	0.5880	0.1912	0.0028
303.15	−0.6241	−0.3483	0.5892	0.1472	0.0030
308.15	−0.6019	−0.4002	0.5887	0.0927	0.0031
313.15	−0.5745	−0.4594	0.5878	0.0565	0.0030
Methanol (1) + Benzene (2)					
288.15	−0.0279	−0.1247	0.1181	−0.0942	0.0007
293.15	−0.0251	−0.1383	0.1352	−0.1187	0.0009
298.15	−0.0171	−0.1541	0.1550	−0.1481	0.0011
303.15	−0.0048	−0.1736	0.1782	−0.1770	0.0014
308.15	0.0135	−0.1940	0.2059	−0.2143	0.0016
313.15	0.0380	−0.2295	0.2385	−0.2130	0.0022
Chloroform (1) + Benzene (2)					
288.15	0.7842	−0.1024	0.1571	−0.1376	0.0030
293.15	0.7441	−0.1042	0.1628	−0.1134	0.0029
298.15	0.7064	−0.1177	0.1667	−0.0627	0.0028
303.15	0.6704	−0.0970	0.1730	−0.0863	0.0027
308.15	0.6348	−0.1112	0.1761	−0.0334	0.0025
313.15	0.5980	−0.1204	0.2074	0.0227	0.0030

Table 5. Parameters $B_p/10^{-9}$ m^3·J^{-1} of Equation 4 and the Corresponding rmsd $\sigma/10^{-6}$ m^3·mol^{-1} for the Methanol (1) + Chloroform (2) + Benzene (3) System

	T/K					
	288.15	293.15	298.15	303.15	308.15	313.15
B_1	0.108	0.218	0.306	0.418	0.470	0.540
B_2	−4.430	−3.448	−2.929	−2.159	−2.103	−1.446
B_3	−1.946	−1.947	−1.745	−1.794	−1.500	−1.237
B_4	12.387	9.904	8.591	7.071	6.967	5.180
B_5	2.597	2.924	2.292	2.774	1.467	0.355
B_6	4.587	4.599	5.032	4.577	5.501	5.431
B_7	−9.861	−7.785	−6.627	−5.611	−5.382	−4.006
B_8	−0.492	−0.940	−0.522	−0.953	0.134	1.219
B_9	−10.020	−10.294	−11.092	−10.511	−11.896	−11.534
σ	0.0039	0.0035	0.0035	0.0036	0.0036	0.0040

where x_1, x_2, and x_3 are mole fractions of the ternary system; V^E_{12}, V^E_{13}, and V^E_{23} represent the excess molar volumes calculated using eq 2 and ternary compositions x_i and x_j; and B_0, B_1, ..., B_8 are the adjustable parameters of ternary contribution obtained from ternary experimental V^E data. These fitted parameters of eq 4 along with the corresponding rmsd, σ, calculated according to eq 3, are given in Table 5.

Supporting Information Available:

Figures S1 to S4 show the V^E data for the binary systems methanol (1) + chloroform (2) for the following investigated temperatures: 288.15, 298.15, and 308.15 K (Figure S1); experimental V^E values at 303.15 K and fitted lines of constant (x_1/x_3) obtained using eq 4 for the ternary system (Figure S2); isolines of the excess molar volume for the ternary system at 288.15 (Figure S3a) and 313.15 K (Figure S3b); and three-dimensional ternary V^E representation of the investigated mixture at 303.15 K generated by eq 4, respectively (Figure S4). This information is available free of charge via the Internet at http: //pubs.acs.org.

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