Densities and Excess Molar Volumes of the Binary 1-Propanol + Chloroform and 1-Propanol + Benzene and Ternary 1-Propanol + Chloroform + Benzene Mixtures at (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K

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Densities ρ and excess molar volumes V^E of the binary 1-propanol + chloroform and 1-propanol + benzene and ternary 1-propanol + chloroform + benzene mixtures have been determined. Experimental ρ measurements have been performed 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 correlated by the Redlich−Kister (for binary data) and Nagata−Tamura (for ternary data) equations.

Introduction

This paper is part of our research of the volumetric properties[1−3] of binaries and multicomponent mixtures containing different alcohols, chloroform and benzene, which have great importance as nonelectrolyte solvents in various industries.[1−3]

In the present work, densities ρ for the ternary system of 1-propanol + chloroform + benzene and binaries 1-propanol + chloroform and 1-propanol + benzene at temperatures (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K and atmospheric pressure have been measured. The related property, excess molar volume V^E, was calculated from the measured ρ data.

The Redlich−Kister equation was used for binary data correlation, and the Nagata and Tamura[4] equation was used for ternary V^E data correlation.

For the binary mixtures 1-propanol + chloroform and 1-propanol + benzene, the ρ and V^E literature data cover only single temperatures, 303.15 K[5] and 298.15 K,[6,7] respectively. In the currently published articles, no values of V^E for those binary systems have been found for the entire temperature range studied here. Also, for the investigated ternary system, literature data are not available.

Experimental Section

Chemicals. 1-Propanol (Merck) was supplied with 99.5% purity (p.a.). Chloroform (stabilized with amylene) was supplied by Riedel-de Haën with a purity of 99.8 %, and benzene was supplied by Aldrich with a purity of 99.9 % (HPLC). Table 1 lists the measured densities of 1-propanol, chloroform, and benzene, which agree to within ± 0.09 kg·m^{-3} with most of the corresponding literature values.[6−9]

Measurements. Densities ρ of the ternary 1-propanol + chloroform + benzene, binaries 1-propanol + chloroform and 1-propanol + benzene, and the 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}. Detailed explanation of the experimental procedure has been given previously.[1−3] For the mixture preparation, 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}, and the average uncertainty in excess molar volume is estimated to be ± 3·10^{-9} m^3·mol^{-1}.

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

	ρ·10^{-3}/(kg·m^{-3})	
component	exptl	lit.
1-propanol	0.799692	0.799543,[a] 0.79962,[b] 0.79960[d]
benzene	0.873582	0.87365,[a] 0.87373,[b] 0.87360[d]
chloroform	1.479148	1.47919,[c] 1.47970[d]

[a] Tanaka and Yokoyama.[6] [b] Singh et al.[7] [c] Francesconi et al.[8] [d] Riddick et al.[9]

Results and Discussion

The excess molar volumes V^E were calculated using the equation

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

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 1-propanol + chloroform and 1-propanol + benzene and the ternary 1-propanol + chloroform + benzene systems. Experimental results for the third binary system chloroform + benzene were presented in our previous paper.[1]

Data for the binary mixtures were correlated with the Redlich−Kister (RK) polynomial

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

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

x_1	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}	x_1	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}	x_1	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}	x_1	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}
1-Propanol (1) + Chloroform (2)											
T = 288.15 K											
0.0000	1.498077	0.0000	0.2999	1.300431	0.0241	0.5497	1.132238	−0.1296	0.7998	0.956019	−0.1875
0.0493	1.465276	0.0497	0.3493	1.267608	−0.0022	0.5999	1.097622	−0.1582	0.8503	0.919243	−0.1660
0.0992	1.432559	0.0634	0.4004	1.233486	−0.0348	0.6497	1.062780	−0.1696	0.9002	0.882470	−0.1280
0.1499	1.399065	0.0797	0.4502	1.200076	−0.0732	0.7001	1.027344	−0.1872	0.9500	0.845487	−0.0846
0.2002	1.365960	0.0764	0.5001	1.166153	−0.0995	0.7499	0.991931	−0.1942	1.0000	0.807690	0.0000
0.2496	1.333594	0.0516									
T = 293.15 K											
0.0000	1.488638	0.0000	0.2999	1.292459	0.0416	0.5497	1.125658	−0.1119	0.7998	0.950913	−0.1797
0.0493	1.456029	0.0559	0.3493	1.259917	0.0153	0.5999	1.091330	−0.1415	0.8503	0.914435	−0.1610
0.0992	1.423544	0.0734	0.4004	1.226067	−0.0164	0.6497	1.056788	−0.1550	0.9002	0.877949	−0.1255
0.1499	1.390299	0.0928	0.4502	1.192931	−0.0545	0.7001	1.021648	−0.1745	0.9500	0.841239	−0.0839
0.2002	1.357456	0.0915	0.5001	1.159294	−0.0814	0.7499	0.986531	−0.1839	1.0000	0.803703	0.0000
0.2496	1.325352	0.0680									
T = 298.15 K											
0.0000	1.479148	0.0000	0.2999	1.284429	0.0604	0.5497	1.119033	−0.0933	0.7998	0.945767	−0.1709
0.0493	1.446744	0.0616	0.3493	1.252163	0.0345	0.5999	1.084995	−0.1240	0.8503	0.909588	−0.1550
0.0992	1.414474	0.0840	0.4004	1.218593	0.0034	0.6497	1.050746	−0.1389	0.9002	0.873397	−0.1226
0.1499	1.381481	0.1064	0.4502	1.185736	−0.0348	0.7001	1.015906	−0.1606	0.9500	0.836960	−0.0827
0.2002	1.348896	0.1075	0.5001	1.152383	−0.0620	0.7499	0.981083	−0.1721	1.0000	0.799692	0.0000
0.2496	1.317054	0.0854									
T = 303.15 K											
0.0000	1.469612	0.0000	0.2999	1.276342	0.0804	0.5497	1.112349	−0.0729	0.7998	0.940572	−0.1608
0.0493	1.437408	0.0677	0.3493	1.244351	0.0550	0.5999	1.078605	−0.1049	0.8503	0.904699	−0.1482
0.0992	1.405354	0.0951	0.4004	1.211064	0.0244	0.6497	1.044651	−0.1214	0.9002	0.868803	−0.1188
0.1499	1.372606	0.1212	0.4502	1.178484	−0.0135	0.7001	1.010111	−0.1451	0.9500	0.832652	−0.0817
0.2002	1.340276	0.1248	0.5001	1.145417	−0.0411	0.7499	0.975586	−0.1591	1.0000	0.795650	0.0000
0.2496	1.308695	0.1044									
T = 308.15 K											
0.0000	1.460025	0.0000	0.2999	1.268188	0.1022	0.5497	1.105602	−0.0507	0.7998	0.935323	−0.1491
0.0493	1.428010	0.0746	0.3493	1.236471	0.0775	0.5999	1.072151	−0.0837	0.8503	0.899757	−0.1399
0.0992	1.396171	0.1072	0.4004	1.203464	0.0477	0.6497	1.038495	−0.1019	0.9002	0.864163	−0.1140
0.1499	1.363670	0.1370	0.4502	1.171164	0.0098	0.7001	1.004259	−0.1280	0.9500	0.828298	−0.0796
0.2002	1.331595	0.1433	0.5001	1.138385	−0.0183	0.7499	0.970031	−0.1442	1.0000	0.791576	0.0000
0.2496	1.300271	0.1248									
T = 313.15 K											
0.0000	1.450413	0.0000	0.2999	1.260011	0.1240	0.5497	1.098810	−0.0272	0.7998	0.930030	−0.1366
0.0493	1.418578	0.0822	0.3493	1.228548	0.1012	0.5999	1.065649	−0.0612	0.8503	0.894778	−0.1314
0.0992	1.386950	0.1203	0.4004	1.195826	0.0717	0.6497	1.032308	−0.0825	0.9002	0.859496	−0.1100
0.1499	1.354698	0.1535	0.4502	1.163793	0.0347	0.7001	0.998364	−0.1100	0.9500	0.823912	−0.0778
0.2002	1.322858	0.1639	0.5001	1.131315	0.0053	0.7499	0.964415	−0.1271	1.0000	0.787466	0.0000
0.2496	1.291797	0.1469									
1-Propanol (1) + Benzene (2)											
T = 288.15 K											
0.0000	0.884246	0.0000	0.2186	0.868541	0.1085	0.5023	0.848393	0.0648	0.8016	0.825211	−0.0127
0.0220	0.882511	0.0311	0.2385	0.867148	0.1095	0.6035	0.840846	0.0371	0.8447	0.821474	−0.0064
0.0557	0.880030	0.0589	0.3046	0.862546	0.1040	0.6600	0.836494	0.0234	0.8981	0.816954	−0.0164
0.0984	0.876959	0.0834	0.3993	0.855836	0.0900	0.7035	0.833115	0.0099	0.9495	0.812375	−0.0128
0.1632	0.872435	0.0995	0.4505	0.852174	0.0770	0.7453	0.829801	−0.0015	1.0000	0.807690	0.0000
T = 293.15 K											
0.0000	0.878918	0.0000	0.2186	0.863367	0.1212	0.5023	0.843581	0.0772	0.8016	0.820875	−0.0072
0.0220	0.877177	0.0347	0.2385	0.861999	0.1222	0.6035	0.836186	0.0476	0.8447	0.817209	−0.0018
0.0557	0.874714	0.0652	0.3046	0.857468	0.1178	0.6600	0.831916	0.0334	0.8981	0.812786	−0.0137
0.0984	0.871673	0.0922	0.3993	0.850881	0.1035	0.7035	0.828615	0.0180	0.9495	0.808313	−0.0129
0.1632	0.867203	0.1110	0.4505	0.847288	0.0901	0.7453	0.825366	0.0059	1.0000	0.803703	0.0000
T = 298.15 K											
0.0000	0.873582	0.0000	0.2186	0.858172	0.1351	0.5023	0.838736	0.0915	0.8016	0.816507	−0.0006
0.0220	0.871937	0.0280	0.2385	0.856826	0.1363	0.6035	0.831492	0.0600	0.8447	0.812998	−0.0042
0.0557	0.869383	0.0722	0.3046	0.852368	0.1328	0.6600	0.827312	0.0443	0.8981	0.808589	−0.0103
0.0984	0.866369	0.1020	0.3993	0.845896	0.1188	0.7035	0.824081	0.0277	0.9495	0.804141	−0.0049
0.1632	0.861955	0.1233	0.4505	0.842370	0.1052	0.7453	0.820902	0.0142	1.0000	0.799692	0.0000
T = 303.15 K											
0.0000	0.868233	0.0000	0.2186	0.852950	0.1503	0.5023	0.833856	0.1075	0.8016	0.812105	0.0068
0.0220	0.866489	0.0412	0.2385	0.851625	0.1519	0.6035	0.826762	0.0738	0.8447	0.808593	0.0092
0.0557	0.864034	0.0799	0.3046	0.847234	0.1497	0.6600	0.822690	0.0547	0.8981	0.804360	−0.0066
0.0984	0.861047	0.1124	0.3993	0.840877	0.1359	0.7035	0.819512	0.0386	0.9495	0.800008	−0.0033
0.1632	0.856682	0.1368	0.4505	0.837417	0.1219	0.7453	0.816400	0.0239	1.0000	0.795650	0.0000

Table 2. (Continued)

x_1	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}	x_1	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}	x_1	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}	x_1	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}
1-Propanol (1) + Benzene (2)											
$T = 308.15$ K											
0.0000	0.862871	0.0000	0.2186	0.847699	0.1672	0.5023	0.828935	0.1257	0.8016	0.807610	0.0206
0.0220	0.861124	0.0447	0.2385	0.846396	0.1690	0.6035	0.821989	0.0898	0.8447	0.804229	0.0161
0.0557	0.858669	0.0879	0.3046	0.842067	0.1685	0.6600	0.817981	0.0715	0.8981	0.800093	−0.0021
0.0984	0.855699	0.1242	0.3993	0.835823	0.1548	0.7035	0.814900	0.0512	0.9495	0.795838	−0.0010
0.1632	0.851380	0.1520	0.4505	0.832428	0.1406	0.7453	0.811856	0.0353	1.0000	0.791576	0.0000
$T = 313.15$ K											
0.0000	0.857498	0.0000	0.2186	0.842427	0.1849	0.5023	0.823986	0.1447	0.8016	0.803184	0.0249
0.0220	0.855764	0.0465	0.2385	0.841156	0.1858	0.6035	0.817183	0.1069	0.8447	0.799833	0.0231
0.0557	0.853296	0.0956	0.3046	0.836875	0.1885	0.6600	0.813261	0.0870	0.8981	0.795804	0.0014
0.0984	0.850343	0.1357	0.3993	0.830744	0.1746	0.7035	0.810256	0.0645	0.9495	0.791644	0.0002
0.1632	0.846063	0.1676	0.4505	0.827425	0.1588	0.7453	0.807285	0.0466	1.0000	0.787466	0.0000

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

x_1	x_2	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho \cdot 10^{-3}$ / kg·m^{-3}	$V^E \cdot 10^6$ / m^3·mol^{-1}
$T = 288.15$ K											
0.0904	0.0999	0.933453	0.1384	0.3202	0.2000	0.979271	0.1553	0.7195	0.1001	0.895228	−0.0587
0.0799	0.2003	0.991320	0.1900	0.2802	0.2999	1.041837	0.1690	0.6398	0.2000	0.964014	−0.0612
0.0694	0.3000	1.049946	0.2204	0.2393	0.4008	1.105561	0.1776	0.5600	0.2998	1.032007	−0.0421
0.0584	0.4012	1.110820	0.2243	0.2002	0.4997	1.168705	0.1682	0.4800	0.4001	1.099843	−0.0190
0.0489	0.5009	1.171945	0.2136	0.1593	0.6014	1.234025	0.1677	0.4005	0.4994	1.166399	0.0129
0.0399	0.6005	1.234259	0.1936	0.1195	0.7011	1.298880	0.1493	0.3200	0.5990	1.232696	0.0444
0.0288	0.7001	1.297840	0.1661	0.0796	0.8002	1.364052	0.1114	0.2397	0.7000	1.299560	0.0682
0.0206	0.7991	1.362605	0.1151	0.0386	0.9009	1.431137	0.0678	0.1600	0.7987	1.364693	0.0773
0.1798	0.1000	0.928064	0.1553	0.5399	0.0996	0.906202	0.0453	0.0805	0.8985	1.430432	0.0700
0.1598	0.1999	0.987100	0.1920	0.4795	0.2003	0.971803	0.0702	0.8095	0.1003	0.889382	−0.1082
0.1406	0.3001	1.047255	0.2108	0.4197	0.3004	1.037330	0.0704	0.7203	0.2002	0.960162	−0.1283
0.1195	0.4002	1.108333	0.2221	0.3609	0.3993	1.101825	0.0915	0.6294	0.3005	1.030311	−0.1238
0.0995	0.5002	1.170497	0.2124	0.2994	0.5003	1.167813	0.1086	0.5393	0.3999	1.098574	−0.0859
0.0803	0.6001	1.233561	0.1965	0.2400	0.6004	1.233271	0.1207	0.4502	0.5009	1.166970	−0.0364
0.0592	0.7003	1.297986	0.1666	0.1788	0.7007	1.299164	0.1166	0.3602	0.5993	1.233025	0.0088
0.0411	0.7994	1.363010	0.1173	0.1200	0.7995	1.364377	0.0976	0.2696	0.6992	1.299546	0.0389
0.0213	0.8984	1.429089	0.0624	0.0595	0.9001	1.431623	0.0729	0.1792	0.8001	1.366000	0.0701
0.3601	0.1000	0.917333	0.1218								
$T = 293.15$ K											
0.0904	0.0999	0.927843	0.1431	0.3202	0.2000	0.973531	0.1644	0.7195	0.1001	0.890397	−0.0516
0.0799	0.2003	0.985368	0.1914	0.2802	0.2999	1.035680	0.1767	0.6398	0.2000	0.958673	−0.0517
0.0694	0.3000	1.043635	0.2195	0.2393	0.4008	1.098961	0.1848	0.5600	0.2998	1.026141	−0.0300
0.0584	0.4012	1.104124	0.2218	0.2002	0.4997	1.161655	0.1751	0.4800	0.4001	1.093446	−0.0052
0.0489	0.5009	1.164851	0.2101	0.1593	0.6014	1.226498	0.1745	0.4005	0.4994	1.159477	0.0275
0.0399	0.6005	1.226743	0.1901	0.1195	0.7011	1.290878	0.1555	0.3200	0.5990	1.225242	0.0593
0.0288	0.7001	1.289881	0.1628	0.0796	0.8002	1.355569	0.1166	0.2397	0.7000	1.291577	0.0821
0.0206	0.7991	1.354179	0.1128	0.0386	0.9009	1.422174	0.0706	0.1600	0.7987	1.356193	0.0894
0.1798	0.1000	0.922531	0.1632	0.5399	0.0996	0.901101	0.0555	0.0805	0.8985	1.421438	0.0781
0.1598	0.1999	0.981211	0.1967	0.4795	0.2003	0.966250	0.0803	0.8095	0.1003	0.884699	−0.1033
0.1406	0.3001	1.040983	0.2139	0.4197	0.3004	1.031306	0.0809	0.7203	0.2002	0.954933	−0.1193
0.1195	0.4002	1.101662	0.2238	0.3609	0.3993	1.095327	0.1024	0.6294	0.3005	1.024523	−0.1114
0.0995	0.5002	1.163402	0.2138	0.2994	0.5003	1.160819	0.1197	0.5393	0.3999	1.092235	−0.0711
0.0803	0.6001	1.226036	0.1972	0.2400	0.6004	1.225777	0.1318	0.4502	0.5009	1.160075	−0.0200
0.0592	0.7003	1.290003	0.1672	0.1788	0.7007	1.291165	0.1270	0.3602	0.5993	1.225589	0.0254
0.0411	0.7994	1.354561	0.1179	0.1200	0.7995	1.355881	0.1066	0.2696	0.6992	1.291571	0.0545
0.0213	0.8984	1.420159	0.0627	0.0595	0.9001	1.422637	0.0785	0.1792	0.8001	1.357490	0.0838
0.3601	0.1000	0.911996	0.1325								
$T = 298.15$ K											
0.0904	0.0999	0.922211	0.1488	0.3202	0.2000	0.967756	0.1749	0.7195	0.1001	0.885527	−0.0430
0.0799	0.2003	0.979390	0.1937	0.2802	0.2999	1.029478	0.1864	0.6398	0.2000	0.953286	−0.0404
0.0694	0.3000	1.037297	0.2193	0.2393	0.4008	1.092316	0.1936	0.5600	0.2998	1.020231	−0.0166
0.0584	0.4012	1.097397	0.2199	0.2002	0.4997	1.154561	0.1832	0.4800	0.4001	1.086998	0.0103
0.0489	0.5009	1.157720	0.2074	0.1593	0.6014	1.218926	0.1822	0.4005	0.4994	1.152499	0.0439
0.0399	0.6005	1.219191	0.1869	0.1195	0.7011	1.282827	0.1626	0.3200	0.5990	1.217736	0.0754
0.0288	0.7001	1.281882	0.1597	0.0796	0.8002	1.347040	0.1222	0.2397	0.7000	1.283536	0.0974
0.0206	0.7991	1.345713	0.1104	0.0386	0.9009	1.413163	0.0736	0.1600	0.7987	1.347639	0.1024
0.1798	0.1000	0.916970	0.1727	0.5399	0.0996	0.895964	0.0673	0.0805	0.8985	1.412398	0.0864
0.1598	0.1999	0.975290	0.2028	0.4795	0.2003	0.960654	0.0923	0.8095	0.1003	0.879981	−0.0973
0.1406	0.3001	1.034674	0.2184	0.4197	0.3004	1.025238	0.0930	0.7203	0.2002	0.949662	−0.1090
0.1195	0.4002	1.094950	0.2269	0.3609	0.3993	1.088781	0.1150	0.6294	0.3005	1.018688	−0.0974
0.0995	0.5002	1.156268	0.2160	0.2994	0.5003	1.153774	0.1324	0.5393	0.3999	1.085845	−0.0547
0.0803	0.6001	1.218464	0.1989	0.2400	0.6004	1.218232	0.1443	0.4502	0.5009	1.153129	−0.0023

Table 3. (Continued)

x_1	x_2	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}	x_1	x_2	$\rho\cdot10^{-3}$ / kg·m^{-3}	$V^E\cdot10^6$ / m^3·mol^{-1}
					$T = 298.15$ K						
0.0592	0.7003	1.281979	0.1681	0.1788	0.7007	1.283116	0.1384	0.3602	0.5993	1.218100	0.0434
0.0411	0.7994	1.346069	0.1186	0.1200	0.7995	1.347336	0.1161	0.2696	0.6992	1.283538	0.0715
0.0213	0.8984	1.411186	0.0629	0.0595	0.9001	1.413604	0.0843	0.1792	0.8001	1.348928	0.0982
0.3601	0.1000	0.906623	0.1451								
					$T = 303.15$ K						
0.0904	0.0999	0.916556	0.1552	0.3202	0.2000	0.961937	0.1874	0.7195	0.1001	0.880614	−0.0330
0.0799	0.2003	0.973386	0.1968	0.2802	0.2999	1.023235	0.1974	0.6398	0.2000	0.947853	−0.0276
0.0694	0.3000	1.030928	0.2198	0.2393	0.4008	1.085625	0.2038	0.5600	0.2998	1.014264	−0.0010
0.0584	0.4012	1.090634	0.2188	0.2002	0.4997	1.147416	0.1928	0.4800	0.4001	1.080497	0.0273
0.0489	0.5009	1.150556	0.2049	0.1593	0.6014	1.211301	0.1913	0.4005	0.4994	1.145468	0.0616
0.0399	0.6005	1.211599	0.1842	0.1195	0.7011	1.274726	0.1706	0.3200	0.5990	1.210172	0.0932
0.0288	0.7001	1.273842	0.1571	0.0796	0.8002	1.338459	0.1286	0.2397	0.7000	1.275437	0.1141
0.0206	0.7991	1.337201	0.1084	0.0386	0.9009	1.404107	0.0767	0.1600	0.7987	1.339031	0.1164
0.1798	0.1000	0.911380	0.1834	0.5399	0.0996	0.890785	0.0809	0.0805	0.8985	1.403305	0.0954
0.1598	0.1999	0.969334	0.2104	0.4795	0.2003	0.955012	0.1060	0.8095	0.1003	0.875219	−0.0902
0.1406	0.3001	1.028329	0.2240	0.4197	0.3004	1.019115	0.1073	0.7203	0.2002	0.944341	−0.0972
0.1195	0.4002	1.088202	0.2308	0.3609	0.3993	1.082184	0.1292	0.6294	0.3005	1.012799	−0.0818
0.0995	0.5002	1.149095	0.2190	0.2994	0.5003	1.146677	0.1466	0.5393	0.3999	1.079395	−0.0363
0.0803	0.6001	1.210853	0.2012	0.2400	0.6004	1.210636	0.1580	0.4502	0.5009	1.146124	0.0171
0.0592	0.7003	1.273910	0.1698	0.1788	0.7007	1.275013	0.1509	0.3602	0.5993	1.210552	0.0629
0.0411	0.7994	1.337532	0.1197	0.1200	0.7995	1.338736	0.1267	0.2696	0.6992	1.275448	0.0898
0.0213	0.8984	1.402166	0.0634	0.0595	0.9001	1.404518	0.0907	0.1792	0.8001	1.340308	0.1139
0.3601	0.1000	0.901213	0.1594								
					$T = 308.15$ K						
0.0904	0.0999	0.910870	0.1631	0.3202	0.2000	0.956070	0.2022	0.7195	0.1001	0.875655	−0.0214
0.0799	0.2003	0.967348	0.2011	0.2802	0.2999	1.016940	0.2106	0.6398	0.2000	0.942365	−0.0128
0.0694	0.3000	1.024523	0.2215	0.2393	0.4008	1.078883	0.2158	0.5600	0.2998	1.008242	0.0164
0.0584	0.4012	1.083837	0.2183	0.2002	0.4997	1.140217	0.2041	0.4800	0.4001	1.073937	0.0463
0.0489	0.5009	1.143352	0.2032	0.1593	0.6014	1.203624	0.2017	0.4005	0.4994	1.138374	0.0814
0.0399	0.6005	1.203961	0.1823	0.1195	0.7011	1.266572	0.1796	0.3200	0.5990	1.202546	0.1126
0.0288	0.7001	1.265755	0.1549	0.0796	0.8002	1.329827	0.1356	0.2397	0.7000	1.267277	0.1322
0.0206	0.7991	1.328641	0.1068	0.0386	0.9009	1.394996	0.0804	0.1600	0.7987	1.330363	0.1315
0.1798	0.1000	0.905754	0.1959	0.5399	0.0996	0.885556	0.0969	0.0805	0.8985	1.394159	0.1048
0.1598	0.1999	0.963342	0.2194	0.4795	0.2003	0.949318	0.1220	0.8095	0.1003	0.870407	−0.0814
0.1406	0.3001	1.021942	0.2312	0.4197	0.3004	1.012942	0.1235	0.7203	0.2002	0.938966	−0.0835
0.1195	0.4002	1.081409	0.2362	0.3609	0.3993	1.075530	0.1454	0.6294	0.3005	1.006851	−0.0641
0.0995	0.5002	1.141874	0.2234	0.2994	0.5003	1.139520	0.1627	0.5393	0.3999	1.072888	−0.0162
0.0803	0.6001	1.203196	0.2043	0.2400	0.6004	1.202976	0.1736	0.4502	0.5009	1.139058	0.0383
0.0592	0.7003	1.265789	0.1723	0.1788	0.7007	1.266847	0.1651	0.3602	0.5993	1.202940	0.0843
0.0411	0.7994	1.328945	0.1213	0.1200	0.7995	1.330082	0.1380	0.2696	0.6992	1.267291	0.1099
0.0213	0.8984	1.393089	0.0645	0.0595	0.9001	1.395381	0.0974	0.1792	0.8001	1.331625	0.1308
0.3601	0.1000	0.895755	0.1764								
					$T = 313.15$ K						
0.0904	0.0999	0.905168	0.1713	0.3202	0.2000	0.950176	0.2177	0.7195	0.1001	0.870661	−0.0092
0.0799	0.2003	0.961302	0.2049	0.2802	0.2999	1.010613	0.2249	0.6398	0.2000	0.936834	0.0033
0.0694	0.3000	1.018099	0.2233	0.2393	0.4008	1.072099	0.2295	0.5600	0.2998	1.002171	0.0356
0.0584	0.4012	1.077023	0.2177	0.2002	0.4997	1.132992	0.2158	0.4800	0.4001	1.067345	0.0658
0.0489	0.5009	1.136134	0.2010	0.1593	0.6014	1.195921	0.2124	0.4005	0.4994	1.131243	0.1020
0.0399	0.6005	1.196308	0.1800	0.1195	0.7011	1.258395	0.1888	0.3200	0.5990	1.194875	0.1335
0.0288	0.7001	1.257635	0.1536	0.0796	0.8002	1.321161	0.1434	0.2397	0.7000	1.259075	0.1515
0.0206	0.7991	1.320062	0.1050	0.0386	0.9009	1.385843	0.0852	0.1600	0.7987	1.321658	0.1475
0.1798	0.1000	0.900114	0.2085	0.5399	0.0996	0.880301	0.1132	0.0805	0.8985	1.384988	0.1143
0.1598	0.1999	0.957328	0.2289	0.4795	0.2003	0.943594	0.1386	0.8095	0.1003	0.865566	−0.0729
0.1406	0.3001	1.015531	0.2390	0.4197	0.3004	1.006734	0.1406	0.7203	0.2002	0.933548	−0.0688
0.1195	0.4002	1.074586	0.2425	0.3609	0.3993	1.068832	0.1633	0.6294	0.3005	1.000851	−0.0447
0.0995	0.5002	1.134622	0.2286	0.2994	0.5003	1.132314	0.1808	0.5393	0.3999	1.066346	0.0044
0.0803	0.6001	1.195496	0.2089	0.2400	0.6004	1.195278	0.1903	0.4502	0.5009	1.131941	0.0613
0.0592	0.7003	1.257645	0.1750	0.1788	0.7007	1.258649	0.1799	0.3602	0.5993	1.195281	0.1071
0.0411	0.7994	1.320321	0.1238	0.1200	0.7995	1.321394	0.1501	0.2696	0.6992	1.259087	0.1315
0.0213	0.8984	1.383982	0.0659	0.0595	0.9001	1.386217	0.1044	0.1792	0.8001	1.322906	0.1485
0.3601	0.1000	0.890271	0.1942								

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's) defined by the equation

$$\sigma = \left(\sum_{i=1}^{m} (V^E_{\text{exptl},i} - V^E_{\text{calcd},i})^2/m\right)^{1/2} \quad (3)$$

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

Comparison of our experimental results of V^E at (298.15 and 303.15) K with data reported previously for the system

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
1-Propanol (1) + Chloroform (2)					
288.15	−0.4029	−1.2198	0.1213	−0.3345	0.0038
293.15	−0.3297	−1.2381	0.1176	−0.3895	0.0037
298.15	−0.2524	−1.2577	0.1159	−0.4321	0.0036
303.15	−0.1679	−1.2757	0.1163	−0.4908	0.0037
308.15	−0.0765	−1.2990	0.1278	−0.5118	0.0037
313.15	0.0196	−1.3178	0.1325	−0.5739	0.0036
1-Propanol (1) + Benzene (2)					
288.15	0.2557	−0.5044	0.1633	−0.2859	0.0033
293.15	0.3105	−0.5183	0.1636	−0.3371	0.0037
298.15	0.3644	−0.5633	0.1895	−0.3290	0.0030
303.15	0.4238	−0.5996	0.2328	−0.3310	0.0042
308.15	0.4984	−0.6072	0.2595	−0.3941	0.0043
313.15	0.5729	−0.6351	0.2674	−0.4437	0.0044

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 1-Propanol (1) + Chloroform (2) + Benzene (3) System

	T/K					
	288.15	293.15	298.15	303.15	308.15	313.15
B_0	0.586	0.666	0.764	0.858	0.925	0.928
B_1	2.401	2.751	3.293	4.179	4.094	3.725
B_2	−1.105	−0.982	−0.591	−0.754	−0.489	−0.196
B_3	−10.946	−11.292	−12.646	−14.693	−14.183	−13.167
B_4	−2.478	−3.001	−4.320	−3.655	−4.740	−6.784
B_5	2.381	2.575	2.606	1.583	2.518	3.527
B_6	10.511	10.568	11.571	12.874	12.654	11.791
B_7	5.899	6.354	7.411	6.959	7.812	9.975
B_8	1.512	1.167	1.185	3.306	1.703	0.693
σ	0.0039	0.0039	0.0041	0.0040	0.0040	0.0045

1-propanol + benzene at 298.15 K shows excellent agreement with the results reported by Tanaka and Yokoyama[6] (within the uncertainty of V^E determination) and a small discrepancy in comparison to Singh et al.[7] ($0.006 \cdot 10^{-6}$ m^3·mol^{-1} at maximum value). For the binary system 1-propanol + chloroform, V^E−x_1 curves follow the same trend (S-shape), but disagreement is higher, especially in the area of the maximum and minimum ($0.025 \cdot 10^{-6}$ m^3·mol^{-1} and $0.069 \cdot 10^{-6}$ m^3·mol^{-1}, respectively).

The V^E data for ternary system were correlated by the Nagata and Tamura[4] model

$$V^E_{123}/10^{-6}\ \mathrm{m^3 \cdot mol^{-1}} = V^E_{12} + V^E_{13} + V^E_{23} + x_1x_2x_3RT(B_0 - B_1x_1 - B_2x_2 - B_3x_1^2 - B_4x_2^2 - B_5x_1x_2 - B_6x_1^3 - B_7x_2^3 - B_8x_1^2x_2) \quad (4)$$

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 1-propanol (1) + chloroform (2) (Figure S1a) and 1-propanol (1) + benzene (Figure S1b) for the investigated temperatures (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K; experimental V^E values at 303.15 K and fitted lines of constants (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 K (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) (4 pages). This material is available free of charge via the Internet at http://pubs.acs.org.

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