Densities and Excess Molar Volumes of 2-Butanol + Cyclohexanamine + Heptane and 2-Butanol + *n*-Heptane at Temperatures between (288.15 and 323.15) K

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The density ρ and excess molar volumes V^E for 2-butanol + cyclohexanamine + heptane and 2-butanol + heptane have been determined at temperatures of (288.15, 293.15, 298.15, 303.15, 308.15, 313.15, 318.15, and 323.15) K at a pressure of 0.1 MPa with an Anton Paar DMA 5000 vibrating tube densimeter. Excess molar volumes V^E were determined and fit to the Redlich−Kister equation for the binary mixture and the Nagata−Tamura equation for the ternary mixture.

Introduction

This paper is continuation of our research of the volumetric properties of multicomponent mixtures containing alcohols (methanol, ethanol, propanol, and butanol) with various industrially important organic compounds.[1–5]

In the present work experimental measurements of density ρ, as well as calculated excess molar volume, of 2-butanol + cyclohexanamine + heptane and 2-butanol + heptane at eight temperatures of (288.15, 293.15, 298.15, 303.15, 308.15, 313.15, 318.15, and 323.15) K at a pressure of 0.1 MPa are reported.

As it was already mentioned,[4,5] bearing in mind very complex molecular interactions present in the mixtures of alcohols with amines and/or alkanes, as well as their very diverse industrial utilization, the thermodynamic investigation of these compounds and their mixtures is of great interest.

Correlation of the binary V^E data determined was performed for the binary mixture with the Redlich−Kister (RK)[6] equation, while the Nagata and Tamura[7] equation was used for the ternary data.

To the best of our knowledge, literature data are not available for the investigated ternary mixture, while for 2-butanol + heptane the ρ and V^E the literature data are reported only at a temperature of 298.15 K.[8]

Experimental Section

Chemicals. 2-Butanol and cyclohexanamine were supplied by Merck with a mass fraction purity > 0.99, while heptane was supplied by Fluka with a mass fraction purity of 0.995. Chemicals were kept in brown bottles under inert nitrogen atmosphere and ultrasonically degassed before preparing the mixture. Table 1 lists the densities measured for pure 2-butanol, cyclohexanamine, and heptane, which agree to within ± $1.5 \cdot 10^{-5}$ with the literature values.[9–11]

Measurements. Densities ρ of the ternary and binary mixtures and corresponding pure substances were measured with an Anton Paar DMA 5000 digital vibrating U-tube densimeter (with automatic viscosity correction) having a stated uncertainty of ± $5 \cdot 10^{-6}$ g·cm^{-3}. The temperature in the cell was regulated to ± 0.001 K with a built-in solid-state thermostat. The temperature was measured by two integrated platinum resistance thermometers with a nominal resistance of 100 Ω and uncertainty of ± 0.01 K; temperature stability was better than ± 0.002 K. A detailed explanation of the experimental procedure has been given previously.[1–5] The mixtures were prepared gravimetrically using a Mettler AG 204 balance with a uncertainty of $1 \cdot 10^{-4}$ g. The uncertainty of the mole fraction was less than ± $1 \cdot 10^{-4}$. All molar quantities were based on the International Union of Pure and Applied Chemistry (IUPAC) relative atomic mass table. The experimental uncertainty in the density is about ± $1 \cdot 10^{-5}$ g·cm^{-3}, while the average uncertainty in excess molar volume is estimated to be ± $2 \cdot 10^{-3}$ cm^3·mol^{-1}.

Table 1. Densities ρ of the Pure Components at $T = 298.15$ K[a] and $p = 0.1$ MPa

component	ρ/g·cm^{-3} expt	ρ/g·cm^{-3} lit.
2-butanol	0.802528	0.8026,[b] 0.80254[c]
cyclohexanamine	0.871290	0.87128,[b] 0.87128[d]
n-heptane	0.679494	0.67951,[b] 0.67951[d]

[a] For cyclohexanamine density is given for $T = 288.15$ K. [b] Riddick et al.[9] [c] Resa et al.[10] [d] Timmermans.[11]

Results and Discussion

The excess molar volumes V^E were obtained 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 molar mass, 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 2-butanol + heptane and 2-butanol + cyclohexanamine + heptane, respectively. In our previous papers, the densities of 2-butanol + cyclohexanamine[5] and cyclohexanamine + heptane[4] have been reported.

Data for the binary mixtures were correlated by the RK equation:[6]

$$V^E_{ij}/\text{cm}^3\cdot\text{mol}^{-1} = x_i x_j \sum_{p=0}^{k} A_p (2x_i - 1)^p \quad (2)$$

where the number $(k + 1)$ of adjustable parameters A_p has been evaluated by the F-test.

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Table 2. Densities ρ and Excess Molar Volumes V^E for 2-Butanol (1) + Heptane (2) at T = (288.15 to 323.15) K and p = 0.1 MPa

x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
				T = 288.15 K				
0.0000	0.687954	0.0000	0.4004	0.721346	0.4915	0.8000	0.774103	0.2151
0.0500	0.691106	0.1599	0.5002	0.732429	0.4663	0.8499	0.782463	0.1625
0.1000	0.694641	0.2656	0.5999	0.744751	0.4120	0.8995	0.791187	0.1173
0.1500	0.698486	0.3363	0.6500	0.751547	0.3632	0.9501	0.800691	0.0614
0.2003	0.702573	0.3946	0.7200	0.761590	0.3009	1.0000	0.810689	0.0000
0.3016	0.711547	0.4693						
				T = 293.15 K				
0.0000	0.683733	0.0000	0.4004	0.716970	0.5284	0.8000	0.769827	0.2380
0.0500	0.686813	0.1773	0.5002	0.728035	0.5058	0.8499	0.778238	0.1795
0.1000	0.690325	0.2889	0.5999	0.740362	0.4504	0.8995	0.787015	0.1289
0.1500	0.694158	0.3628	0.6500	0.747174	0.3990	0.9501	0.796583	0.0669
0.2003	0.698236	0.4234	0.7200	0.757255	0.3312	1.0000	0.806646	0.0000
0.3016	0.707194	0.5019						
				T = 298.15 K				
0.0000	0.679494	0.0000	0.4004	0.712546	0.5687	0.8000	0.765479	0.2633
0.0500	0.682487	0.1979	0.5002	0.723591	0.5483	0.8499	0.773935	0.1991
0.1000	0.685970	0.3164	0.5999	0.735917	0.4916	0.8995	0.782767	0.1420
0.1500	0.689789	0.3936	0.6500	0.742739	0.4378	0.9501	0.792396	0.0736
0.2003	0.693854	0.4569	0.7200	0.752851	0.3647	1.0000	0.802528	0.0000
0.3016	0.702791	0.5392						
				T = 303.15 K				
0.0000	0.675229	0.0000	0.4004	0.708073	0.6113	0.8000	0.761053	0.2909
0.0500	0.678127	0.2204	0.5002	0.719095	0.5927	0.8499	0.769552	0.2204
0.1000	0.681576	0.3467	0.5999	0.731411	0.5351	0.8995	0.778434	0.1569
0.1500	0.685376	0.4277	0.6500	0.738239	0.4790	0.9501	0.788125	0.0811
0.2003	0.689427	0.4936	0.7200	0.748373	0.4011	1.0000	0.798326	0.0000
0.3016	0.698341	0.5793						
				T = 308.15 K				
0.0000	0.670941	0.0000	0.4004	0.703542	0.6579	0.8000	0.756541	0.3210
0.0500	0.673731	0.2459	0.5002	0.714540	0.6400	0.8499	0.765080	0.2438
0.1000	0.677138	0.3814	0.5999	0.726839	0.5815	0.8995	0.774010	0.1732
0.1500	0.680913	0.4671	0.6500	0.733670	0.5228	0.9501	0.783761	0.0893
0.2003	0.684946	0.5358	0.7200	0.743821	0.4397	1.0000	0.794030	0.0000
0.3016	0.693835	0.6241						
				T = 313.15 K				
0.0000	0.666621	0.0000	0.4004	0.698952	0.7072	0.8000	0.751943	0.3528
0.0500	0.669301	0.2720	0.5002	0.709925	0.6892	0.8499	0.760519	0.2684
0.1000	0.672659	0.4180	0.5999	0.722202	0.6293	0.8995	0.769495	0.1900
0.1500	0.676402	0.5095	0.6500	0.729030	0.5683	0.9501	0.779299	0.0980
0.2003	0.680415	0.5811	0.7200	0.739190	0.4802	1.0000	0.789632	0.0000
0.3016	0.689275	0.6717						
				T = 318.15 K				
0.0000	0.662273	0.0000	0.4004	0.694299	0.7600	0.8000	0.747257	0.3852
0.0500	0.664835	0.3001	0.5002	0.705243	0.7410	0.8499	0.755863	0.2935
0.1000	0.668131	0.4592	0.5999	0.717496	0.6786	0.8995	0.764879	0.2072
0.1500	0.671840	0.5564	0.6500	0.724317	0.6151	0.9501	0.774738	0.1057
0.2003	0.675830	0.6308	0.7200	0.734479	0.5217	1.0000	0.785117	0.0000
0.3016	0.684650	0.7247						
				T = 323.15 K				
0.0000	0.657896	0.0000	0.4004	0.689584	0.8175	0.8000	0.742488	0.4205
0.0500	0.660336	0.3295	0.5002	0.700502	0.7959	0.8499	0.751116	0.3218
0.1000	0.663562	0.5033	0.5999	0.712720	0.7316	0.8995	0.760166	0.2274
0.1500	0.667230	0.6075	0.6500	0.719533	0.6652	0.9501	0.770073	0.1164
0.2003	0.671188	0.6863	0.7200	0.729690	0.5667	1.0000	0.780515	0.0000
0.3016	0.679969	0.7822						

Adjustable parameters determined at each temperature and the corresponding root-mean-square deviations (rmsd's) are defined by the equation:

$$\sigma = \left(\sum_{i=1}^{m} (V^E_{\mathrm{exp},i} - V^E_{\mathrm{cal},i})^2/m\right)^{1/2} \quad (3)$$

for all binary mixtures studied are given in Table 4. In eq 3 m is the number of experimental data points.

Comparisons of our experimental results of V^E for 2-butanol + heptane at T = 298.15 K with the data reported previously[8] show that our V^E data are in the excellent agreement with the literature data (see Supporting Information).

The V^E for the ternary mixtures were correlated by the Nagata and Tamura[7] equation:

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

where x_1, x_2, and x_3 are mole fractions of the ternary system,

Table 3. Densities ρ and Excess Molar Volumes V^E for 2-Butanol (1) + Cyclohexanamine (2) + Heptane (3) at T = (288.15 to 323.15) K and p = 0.1 MPa

x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
			T = 288.15 K				
0.0000	1.0000	0.871290	0.0000	0.5401	0.0999	0.759947	−0.0041
0.0911	0.1001	0.710007	0.1104	0.4800	0.1999	0.774154	−0.2652
0.0801	0.2002	0.725086	0.0913	0.4201	0.2998	0.787777	−0.4348
0.0678	0.3006	0.740535	0.0968	0.3596	0.4005	0.800845	−0.5114
0.0606	0.3998	0.756821	0.1257	0.3001	0.4997	0.813190	−0.5113
0.0500	0.5000	0.773636	0.1438	0.2400	0.5999	0.825384	−0.4756
0.0403	0.5996	0.791274	0.1435	0.1798	0.6999	0.837312	−0.4154
0.0305	0.6991	0.809738	0.1288	0.1203	0.7994	0.848653	−0.2796
0.0203	0.7997	0.829267	0.1035	0.0602	0.8997	0.860076	−0.1497
0.1801	0.1004	0.718547	0.0790	0.7196	0.1003	0.787305	−0.1382
0.1603	0.2002	0.733819	−0.0174	0.6399	0.2001	0.799581	−0.3980
0.1402	0.3000	0.749159	−0.0417	0.5602	0.2998	0.811179	−0.5998
0.1204	0.3998	0.764832	−0.0302	0.4799	0.3998	0.821670	−0.6897
0.1003	0.4998	0.781023	−0.0174	0.4001	0.4999	0.831599	−0.7199
0.0804	0.5995	0.797800	−0.0148	0.3200	0.5999	0.840535	−0.6583
0.0604	0.6995	0.815200	−0.0109	0.2399	0.7000	0.848947	−0.5515
0.0400	0.7999	0.833199	−0.0014	0.1599	0.8000	0.856858	−0.4053
0.0200	0.8998	0.851862	−0.0002	0.0802	0.8997	0.864148	−0.2042
0.3601	0.1001	0.737428	0.0644	0.8096	0.1003	0.803189	−0.2236
0.3201	0.2000	0.752682	−0.1682	0.7199	0.2000	0.814075	−0.4813
0.2802	0.3001	0.767446	−0.2662	0.6297	0.3002	0.824183	−0.6772
0.2399	0.4001	0.781962	−0.2955	0.5399	0.4002	0.833263	−0.7799
0.2002	0.4999	0.796479	−0.2807	0.4499	0.5001	0.841381	−0.8050
0.1599	0.6002	0.811433	−0.2910	0.3602	0.5995	0.848563	−0.7533
0.1201	0.7000	0.825946	−0.2063	0.2700	0.6998	0.854972	−0.6176
0.0801	0.8000	0.840865	−0.1438	0.1800	0.7997	0.860769	−0.4385
0.0401	0.8998	0.855671	−0.0390	0.0905	0.8991	0.866147	−0.2338
			T = 293.15 K				
0.0000	1.0000	0.866747	0.0000	0.5401	0.0999	0.755625	0.0125
0.0911	0.1001	0.705693	0.1230	0.4800	0.1999	0.769837	−0.2586
0.0801	0.2002	0.720797	0.0915	0.4201	0.2998	0.783451	−0.4347
0.0678	0.3006	0.736242	0.0911	0.3596	0.4005	0.796501	−0.5152
0.0606	0.3998	0.752519	0.1161	0.3001	0.4997	0.808835	−0.5188
0.0500	0.5000	0.769319	0.1316	0.2400	0.5999	0.820979	−0.4807
0.0403	0.5996	0.786935	0.1301	0.1798	0.6999	0.832900	−0.4238
0.0305	0.6991	0.805361	0.1170	0.1203	0.7994	0.844234	−0.2903
0.0203	0.7997	0.824856	0.0927	0.0602	0.8997	0.855610	−0.1571
0.1801	0.1004	0.714222	0.0936	0.7196	0.1003	0.783057	−0.1293
0.1603	0.2002	0.729502	−0.0126	0.6399	0.2001	0.795317	−0.3959
0.1402	0.3000	0.744843	−0.0439	0.5602	0.2998	0.806885	−0.6017
0.1204	0.3998	0.760513	−0.0377	0.4799	0.3998	0.817340	−0.6936
0.1003	0.4998	0.776693	−0.0282	0.4001	0.4999	0.827243	−0.7263
0.0804	0.5995	0.793338	−0.0098	0.3200	0.5999	0.836160	−0.6669
0.0604	0.6995	0.810715	−0.0074	0.2399	0.7000	0.844549	−0.5613
0.0400	0.7999	0.828766	−0.0096	0.1599	0.8000	0.852430	−0.4148
0.0200	0.8998	0.847385	−0.0058	0.0802	0.8997	0.859677	−0.2109
0.3601	0.1001	0.733088	0.0825	0.8096	0.1003	0.799012	−0.2214
0.3201	0.2000	0.748347	−0.1601	0.7199	0.2000	0.809852	−0.4822
0.2802	0.3001	0.763111	−0.2657	0.6297	0.3002	0.819915	−0.6808
0.2399	0.4001	0.777624	−0.3005	0.5399	0.4002	0.828949	−0.7846
0.2002	0.4999	0.792132	−0.2894	0.4499	0.5001	0.837029	−0.8110
0.1599	0.6002	0.807074	−0.3030	0.3602	0.5995	0.844183	−0.7608
0.1201	0.7000	0.821597	−0.2232	0.2700	0.6998	0.850642	−0.6356
0.0801	0.8000	0.836416	−0.1501	0.1800	0.7997	0.856337	−0.4471
0.0401	0.8998	0.851187	−0.0435	0.0905	0.8991	0.861673	−0.2400
			T = 298.15 K				
0.0000	1.0000	0.862207	0.0000	0.5401	0.0999	0.751251	0.0313
0.0911	0.1001	0.701423	0.1233	0.4800	0.1999	0.765482	−0.2515
0.0801	0.2002	0.716478	0.0939	0.4201	0.2998	0.779092	−0.4343
0.0678	0.3006	0.731924	0.0868	0.3596	0.4005	0.792130	−0.5190
0.0606	0.3998	0.748197	0.1072	0.3001	0.4997	0.804458	−0.5264
0.0500	0.5000	0.764986	0.1197	0.2400	0.5999	0.816653	−0.4995
0.0403	0.5996	0.782582	0.1171	0.1798	0.6999	0.828431	−0.4263
0.0305	0.6991	0.800982	0.1041	0.1203	0.7994	0.839801	−0.3003
0.0203	0.7997	0.820439	0.0820	0.0602	0.8997	0.851138	−0.1642
0.1801	0.1004	0.709860	0.1112	0.7196	0.1003	0.778754	−0.1198
0.1603	0.2002	0.725153	−0.0058	0.6399	0.2001	0.791009	−0.3939
0.1402	0.3000	0.740499	−0.0446	0.5602	0.2998	0.802557	−0.6045
0.1204	0.3998	0.756172	−0.0444	0.4799	0.3998	0.812984	−0.6986
0.1003	0.4998	0.772346	−0.0388	0.4001	0.4999	0.822864	−0.7334
0.0804	0.5995	0.788977	−0.0224	0.3200	0.5999	0.831766	−0.6760
0.0604	0.6995	0.806260	−0.0095	0.2399	0.7000	0.840137	−0.5714
0.0400	0.7999	0.824290	−0.0124	0.1599	0.8000	0.847992	−0.4243

Table 3 Continued

x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
0.0200	0.8998	0.842879	−0.0076	0.0802	0.8997	0.855201	−0.2174
0.3601	0.1001	0.728706	0.1030	0.8096	0.1003	0.794772	−0.2186
0.3201	0.2000	0.743977	−0.1512	0.7199	0.2000	0.805592	−0.4851
0.2802	0.3001	0.758745	−0.2642	0.6297	0.3002	0.815611	−0.6854
0.2399	0.4001	0.773262	−0.3053	0.5399	0.4002	0.824604	−0.7903
0.2002	0.4999	0.787765	−0.2981	0.4499	0.5001	0.832652	−0.8178
0.1599	0.6002	0.802696	−0.3146	0.3602	0.5995	0.839785	−0.7691
0.1201	0.7000	0.817186	−0.2331	0.2700	0.6998	0.846213	−0.6434
0.0801	0.8000	0.832029	−0.1662	0.1800	0.7997	0.851890	−0.4551
0.0401	0.8998	0.846733	−0.0524	0.0905	0.8991	0.857190	−0.2459
			$T = 303.15$ K				
0.0000	1.0000	0.857671	0.0000	0.5401	0.0999	0.746823	0.0515
0.0911	0.1001	0.696987	0.1515	0.4800	0.1999	0.761083	−0.2441
0.0801	0.2002	0.712133	0.0966	0.4201	0.2998	0.774696	−0.4341
0.0678	0.3006	0.727584	0.0824	0.3596	0.4005	0.787734	−0.5239
0.0606	0.3998	0.743856	0.0979	0.3001	0.4997	0.800055	−0.5344
0.0500	0.5000	0.760636	0.1076	0.2400	0.5999	0.812215	−0.5058
0.0403	0.5996	0.778216	0.1038	0.1798	0.6999	0.823969	−0.4319
0.0305	0.6991	0.796591	0.0913	0.1203	0.7994	0.835362	−0.3109
0.0203	0.7997	0.816016	0.0710	0.0602	0.8997	0.846659	−0.1709
0.1801	0.1004	0.705459	0.1308	0.7196	0.1003	0.774386	−0.1093
0.1603	0.2002	0.720771	0.0022	0.6399	0.2001	0.786651	−0.3923
0.1402	0.3000	0.736129	−0.0452	0.5602	0.2998	0.798187	−0.6078
0.1204	0.3998	0.751810	−0.0515	0.4799	0.3998	0.808598	−0.7049
0.1003	0.4998	0.767979	−0.0494	0.4001	0.4999	0.818462	−0.7417
0.0804	0.5995	0.784599	−0.0348	0.3200	0.5999	0.827352	−0.6859
0.0604	0.6995	0.801864	−0.0223	0.2399	0.7000	0.835706	−0.5815
0.0400	0.7999	0.819802	−0.0145	0.1599	0.8000	0.843542	−0.4337
0.0200	0.8998	0.838360	−0.0079	0.0802	0.8997	0.850717	−0.2235
0.3601	0.1001	0.724278	0.1252	0.8096	0.1003	0.790465	−0.2156
0.3201	0.2000	0.739569	−0.1413	0.7199	0.2000	0.801274	−0.4880
0.2802	0.3001	0.754347	−0.2625	0.6297	0.3002	0.811267	−0.6914
0.2399	0.4001	0.768872	−0.3100	0.5399	0.4002	0.820230	−0.7977
0.2002	0.4999	0.783374	−0.3067	0.4499	0.5001	0.828255	−0.8265
0.1599	0.6002	0.798098	−0.2960	0.3602	0.5995	0.835368	−0.7786
0.1201	0.7000	0.812804	−0.2492	0.2700	0.6998	0.841797	−0.6554
0.0801	0.8000	0.827609	−0.1790	0.1800	0.7997	0.847441	−0.4645
0.0401	0.8998	0.842441	−0.0842	0.0905	0.8991	0.852707	−0.2519
			$T = 308.15$ K				
0.0000	1.0000	0.853138	0.0000	0.5401	0.0999	0.742337	0.0734
0.0911	0.1001	0.692602	0.1648	0.4800	0.1999	0.756633	−0.2356
0.0801	0.2002	0.707754	0.1014	0.4201	0.2998	0.770260	−0.4338
0.0678	0.3006	0.723217	0.0790	0.3596	0.4005	0.783301	−0.5286
0.0606	0.3998	0.739492	0.0892	0.3001	0.4997	0.795626	−0.5428
0.0500	0.5000	0.756268	0.0955	0.2400	0.5999	0.807806	−0.5197
0.0403	0.5996	0.773833	0.0908	0.1798	0.6999	0.819526	−0.4426
0.0305	0.6991	0.792188	0.0786	0.1203	0.7994	0.830908	−0.3210
0.0203	0.7997	0.811585	0.0601	0.0602	0.8997	0.842175	−0.1774
0.1801	0.1004	0.701012	0.1542	0.7196	0.1003	0.769950	−0.0981
0.1603	0.2002	0.716349	0.0127	0.6399	0.2001	0.782241	−0.3914
0.1402	0.3000	0.731729	−0.0447	0.5602	0.2998	0.793775	−0.6123
0.1204	0.3998	0.747419	−0.0574	0.4799	0.3998	0.804176	−0.7122
0.1003	0.4998	0.763592	−0.0599	0.4001	0.4999	0.814030	−0.7510
0.0804	0.5995	0.780207	−0.0477	0.3200	0.5999	0.822912	−0.6961
0.0604	0.6995	0.797455	−0.0351	0.2399	0.7000	0.831260	−0.5924
0.0400	0.7999	0.815428	−0.0345	0.1599	0.8000	0.839080	−0.4434
0.0200	0.8998	0.834008	−0.0321	0.0802	0.8997	0.846230	−0.2298
0.3601	0.1001	0.719794	0.1511	0.8096	0.1003	0.786086	−0.2127
0.3201	0.2000	0.735115	−0.1293	0.7199	0.2000	0.796899	−0.4920
0.2802	0.3001	0.749913	−0.2600	0.6297	0.3002	0.806877	−0.6989
0.2399	0.4001	0.764450	−0.3141	0.5399	0.4002	0.815817	−0.8063
0.2002	0.4999	0.778958	−0.3152	0.4499	0.5001	0.823823	−0.8359
0.1599	0.6002	0.793889	−0.3388	0.3602	0.5995	0.830923	−0.7885
0.1201	0.7000	0.808329	−0.2540	0.2700	0.6998	0.837356	−0.6672
0.0801	0.8000	0.823104	−0.1810	0.1800	0.7997	0.842973	−0.4733
0.0401	0.8998	0.837779	−0.0653	0.0905	0.8991	0.848215	−0.2577
			$T = 313.15$ K				
0.0000	1.0000	0.848607	0.0000	0.5401	0.0999	0.737789	0.0963
0.0911	0.1001	0.688169	0.1815	0.4800	0.1999	0.752131	−0.2271
0.0801	0.2002	0.703341	0.1069	0.4201	0.2998	0.765778	−0.4336
0.0678	0.3006	0.718822	0.0754	0.3596	0.4005	0.778832	−0.5341
0.0606	0.3998	0.735103	0.0803	0.3001	0.4997	0.791168	−0.5522
0.0500	0.5000	0.751878	0.0832	0.2400	0.5999	0.803387	−0.5363
0.0403	0.5996	0.769434	0.0771	0.1798	0.6999	0.815146	−0.4654
0.0305	0.6991	0.787773	0.0653	0.1203	0.7994	0.826440	−0.3313

Table 3 Continued

x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
0.0203	0.7997	0.807146	0.0489	0.0602	0.8997	0.837682	−0.1837
0.1801	0.1004	0.696518	0.1799	0.7196	0.1003	0.765440	−0.0864
0.1603	0.2002	0.711888	0.0244	0.6399	0.2001	0.777769	−0.3908
0.1402	0.3000	0.727296	−0.0440	0.5602	0.2998	0.789315	−0.6181
0.1204	0.3998	0.743001	−0.0635	0.4799	0.3998	0.799714	−0.7207
0.1003	0.4998	0.759180	−0.0705	0.4001	0.4999	0.809568	−0.7617
0.0804	0.5995	0.775792	−0.0603	0.3200	0.5999	0.818445	−0.7072
0.0604	0.6995	0.793028	−0.0476	0.2399	0.7000	0.826791	−0.6036
0.0400	0.7999	0.811094	−0.0623	0.1599	0.8000	0.834601	−0.4529
0.0200	0.8998	0.829612	−0.0512	0.0802	0.8997	0.841731	−0.2356
0.3601	0.1001	0.715256	0.1788	0.8096	0.1003	0.781631	−0.2104
0.3201	0.2000	0.730615	−0.1164	0.7199	0.2000	0.792462	−0.4973
0.2802	0.3001	0.745441	−0.2574	0.6297	0.3002	0.802439	−0.7083
0.2399	0.4001	0.759997	−0.3186	0.5399	0.4002	0.811365	−0.8169
0.2002	0.4999	0.774517	−0.3244	0.4499	0.5001	0.819360	−0.8471
0.1599	0.6002	0.789450	−0.3509	0.3602	0.5995	0.826456	−0.8002
0.1201	0.7000	0.803906	−0.2692	0.2700	0.6998	0.832912	−0.6822
0.0801	0.8000	0.818689	−0.1978	0.1800	0.7997	0.838490	−0.4823
0.0401	0.8998	0.833301	−0.0727	0.0905	0.8991	0.843715	−0.2634
			$T = 318.15$ K				
0.0000	1.0000	0.844073	0.0000	0.5401	0.0999	0.733174	0.1207
0.0911	0.1001	0.683702	0.1991	0.4800	0.1999	0.747571	−0.2181
0.0801	0.2002	0.698893	0.1137	0.4201	0.2998	0.761251	−0.4343
0.0678	0.3006	0.714391	0.0735	0.3596	0.4005	0.774326	−0.5408
0.0606	0.3998	0.730686	0.0717	0.3001	0.4997	0.786676	−0.5625
0.0500	0.5000	0.747464	0.0710	0.2400	0.5999	0.798834	−0.5383
0.0403	0.5996	0.765015	0.0633	0.1798	0.6999	0.810612	−0.4701
0.0305	0.6991	0.783345	0.0512	0.1203	0.7994	0.821957	−0.3421
0.0203	0.7997	0.802692	0.0378	0.0602	0.8997	0.833180	−0.1903
0.1801	0.1004	0.691977	0.2085	0.7196	0.1003	0.760857	−0.0756
0.1603	0.2002	0.707374	0.0400	0.6399	0.2001	0.773236	−0.3918
0.1402	0.3000	0.722825	−0.0419	0.5602	0.2998	0.784802	−0.6255
0.1204	0.3998	0.738550	−0.0690	0.4799	0.3998	0.795205	−0.7307
0.1003	0.4998	0.754742	−0.0812	0.4001	0.4999	0.805065	−0.7736
0.0804	0.5995	0.771357	−0.0734	0.3200	0.5999	0.813951	−0.7201
0.0604	0.6995	0.788585	−0.0607	0.2399	0.7000	0.822299	−0.6159
0.0400	0.7999	0.806541	−0.0596	0.1599	0.8000	0.830105	−0.4631
0.0200	0.8998	0.825197	−0.0691	0.0802	0.8997	0.837221	−0.2415
0.3601	0.1001	0.710658	0.2094	0.8096	0.1003	0.777094	−0.2094
0.3198	0.2000	0.726064	−0.1084	0.7199	0.2000	0.787960	−0.5049
0.2802	0.3001	0.740924	−0.2541	0.6297	0.3002	0.797945	−0.7200
0.2402	0.4001	0.755507	−0.3165	0.5399	0.4002	0.806869	−0.8301
0.1998	0.4999	0.770041	−0.3426	0.4499	0.5001	0.814861	−0.8605
0.1599	0.6002	0.784986	−0.3634	0.3602	0.5995	0.821955	−0.8132
0.1201	0.7000	0.799432	−0.2802	0.2700	0.6998	0.828413	−0.6943
0.0801	0.8000	0.814213	−0.2083	0.1800	0.7997	0.833990	−0.4922
0.0401	0.8998	0.828812	−0.0801	0.0905	0.8991	0.839203	−0.2694
			$T = 323.15$ K				
0.0000	1.0000	0.839547	0.0000	0.5401	0.0999	0.728494	0.1481
0.0911	0.1001	0.679102	0.2390	0.4800	0.1999	0.742957	−0.2074
0.0801	0.2002	0.694407	0.1228	0.4201	0.2998	0.756672	−0.4330
0.0678	0.3006	0.709936	0.0715	0.3596	0.4005	0.769780	−0.5466
0.0606	0.3998	0.726247	0.0631	0.3001	0.4997	0.782152	−0.5721
0.0500	0.5000	0.743031	0.0588	0.2400	0.5999	0.794314	−0.5483
0.0403	0.5996	0.760582	0.0493	0.1798	0.6999	0.806033	−0.4703
0.0305	0.6991	0.778902	0.0379	0.1203	0.7994	0.817459	−0.3520
0.0203	0.7997	0.798233	0.0267	0.0602	0.8997	0.828669	−0.1957
0.1801	0.1004	0.687376	0.2432	0.7196	0.1003	0.756194	−0.0618
0.1603	0.2002	0.702828	0.0563	0.6399	0.2001	0.768639	−0.3915
0.1402	0.3000	0.718316	−0.0378	0.5602	0.2998	0.780237	−0.6324
0.1204	0.3998	0.734065	−0.0727	0.4799	0.3998	0.790657	−0.7408
0.1003	0.4998	0.750272	−0.0899	0.4001	0.4999	0.800529	−0.7854
0.0804	0.5995	0.766900	−0.0856	0.3200	0.5999	0.809425	−0.7321
0.0604	0.6995	0.784126	−0.0731	0.2399	0.7000	0.817784	−0.6274
0.0400	0.7999	0.802455	−0.1289	0.1599	0.8000	0.825592	−0.4723
0.0200	0.8998	0.820789	−0.0882	0.0802	0.8997	0.832705	−0.2468
0.3601	0.1001	0.706002	0.2440	0.8096	0.1003	0.772475	−0.2065
0.3201	0.2000	0.721478	−0.0877	0.7199	0.2000	0.783389	−0.5115
0.2802	0.3001	0.736370	−0.2498	0.6297	0.3002	0.793396	−0.7315
0.2399	0.4001	0.750976	−0.3255	0.5399	0.4002	0.802330	−0.8435
0.2002	0.4999	0.765536	−0.3413	0.4499	0.5001	0.810329	−0.8744
0.1599	0.6002	0.780498	−0.3751	0.3602	0.5995	0.817427	−0.8262
0.1201	0.7000	0.794989	−0.2980	0.2700	0.6998	0.823865	−0.7022
0.0801	0.8000	0.809741	−0.2204	0.1800	0.7997	0.829471	−0.5009
0.0401	0.8998	0.824307	−0.0851	0.0905	0.8991	0.834684	−0.2745

Table 4. Parameters A_p of Equation 2 and the Corresponding rmsd's σ for the Binary Mixtures at Temperature T

T	A_0	A_1	A_2	A_3	σ
K	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$
2-Butanol (1) + *n*-Heptane (2)					
288.15	1.8501	−0.8265	0.2905	−0.3317	0.0069
293.15	2.0033	−0.8015	0.3349	−0.5010	0.0082
298.15	2.1678	−0.7769	0.4131	−0.6987	0.0097
303.15	2.3411	−0.7501	0.5158	−0.9149	0.0111
308.15	2.5264	−0.7383	0.6522	−1.1376	0.0125
313.15	2.7203	−0.7330	0.8015	−1.3635	0.0137
318.15	2.9243	−0.7474	0.9704	−1.6003	0.0149
323.15	3.1435	−0.7773	1.1694	−1.8131	0.0159
2-Butanol (1) + Cyclohexanamine (2)[a]					
288.15	−3.4769	−0.4033	0.5327	0.2853	0.0033
293.15	−3.4991	−0.3802	0.5142	0.2381	0.0032
298.15	−3.5225	−0.3719	0.4732	0.2331	0.0032
303.15	−3.5527	−0.3764	0.4321	0.2415	0.0031
308.15	−3.5902	−0.3795	0.3916	0.2257	0.0031
313.15	−3.6483	−0.3995	0.4021	0.2258	0.0036
318.15	−3.6941	−0.4215	0.3044	0.1993	0.0031
323.15	−3.7579	−0.4384	0.2891	0.1649	0.0029
Cyclohexanamine (1) + *n*-Heptane (2)[b]					
288.15	1.2537	−0.5444	0.3720	0.2252	0.0017
293.15	1.2065	−0.5553	0.3288	0.2399	0.0016
298.15	1.1583	−0.5640	0.2953	0.2351	0.0016
303.15	1.1035	−0.5708	0.2718	0.2351	0.0018
308.15	1.0471	−0.5766	0.2592	0.2168	0.0018
313.15	0.9869	−0.5830	0.2406	0.2185	0.0018
318.15	0.9238	−0.5905	0.2248	0.2139	0.0018
323.15	0.8596	−0.5919	0.2151	0.1979	0.0015

[a] Radovic et al.[5] [b] Kijevčanin et al.[4]

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 σ, calculated according to eq 3, are given in Table 5.

Supporting Information Available:

Figures S1 to S4 show the following: the V^E data for the binary system 2-butanol (1) + *n*-heptane (2) (Figure S1a) for all investigated temperatures (288.15, 293.15, 298.15, 303.15, 308.15, 313.15, 318.15, and 323.15) K and a comparison of the experimental values of V^E data at 298.15 K for the same binary system (Figure S1b); 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 303.15 (Figure S3); and a 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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Table 5. Parameters B_p of Equation 4 and the Corresponding rmsd's σ for 2-Butanol (1) + Cyclohexanamine (2) + Heptane (3) at Temperature T

	T/K							
	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15
$B_0/cm^3 \cdot J^{-1}$	$-1.3506 \cdot 10^{-2}$	$-1.3733 \cdot 10^{-2}$	$-1.4511 \cdot 10^{-2}$	$-1.4443 \cdot 10^{-2}$	$-1.4745 \cdot 10^{-2}$	$-1.4808 \cdot 10^{-2}$	$-1.5001 \cdot 10^{-2}$	$-1.4382 \cdot 10^{-2}$
$B_1/cm^3 \cdot J^{-1}$	$-2.0857 \cdot 10^{-2}$	$-2.2579 \cdot 10^{-2}$	$-2.5135 \cdot 10^{-2}$	$-2.5945 \cdot 10^{-2}$	$-2.6045 \cdot 10^{-2}$	$-2.6734 \cdot 10^{-2}$	$-2.6889 \cdot 10^{-2}$	$-2.4239 \cdot 10^{-2}$
$B_2/cm^3 \cdot J^{-1}$	$-2.7848 \cdot 10^{-2}$	$-2.8077 \cdot 10^{-2}$	$-3.0050 \cdot 10^{-2}$	$-2.8119 \cdot 10^{-2}$	$-3.0090 \cdot 10^{-2}$	$-2.9142 \cdot 10^{-2}$	$-2.9883 \cdot 10^{-2}$	$-2.6264 \cdot 10^{-2}$
$B_3/cm^3 \cdot J^{-1}$	$6.4043 \cdot 10^{-3}$	$1.2639 \cdot 10^{-2}$	$1.6274 \cdot 10^{-2}$	$1.9360 \cdot 10^{-2}$	$1.9956 \cdot 10^{-2}$	$2.2068 \cdot 10^{-2}$	$2.2821 \cdot 10^{-2}$	$1.8900 \cdot 10^{-2}$
$B_4/cm^3 \cdot J^{-1}$	$1.4395 \cdot 10^{-2}$	$1.3714 \cdot 10^{-2}$	$1.5003 \cdot 10^{-2}$	$9.3210 \cdot 10^{-3}$	$1.4939 \cdot 10^{-2}$	$1.1149 \cdot 10^{-2}$	$1.3090 \cdot 10^{-2}$	$6.2710 \cdot 10^{-3}$
$B_5/cm^3 \cdot J^{-1}$	$3.0056 \cdot 10^{-2}$	$3.3705 \cdot 10^{-2}$	$3.8327 \cdot 10^{-2}$	$3.9179 \cdot 10^{-2}$	$3.8951 \cdot 10^{-2}$	$4.0036 \cdot 10^{-2}$	$3.9655 \cdot 10^{-2}$	$3.3143 \cdot 10^{-2}$
$B_6/cm^3 \cdot J^{-1}$	$3.2662 \cdot 10^{-3}$	$-9.8526 \cdot 10^{-4}$	$-2.2534 \cdot 10^{-3}$	$-4.5481 \cdot 10^{-3}$	$-4.7581 \cdot 10^{-3}$	$-5.8472 \cdot 10^{-3}$	$-6.5951 \cdot 10^{-3}$	$-4.8864 \cdot 10^{-3}$
$B_7/cm^3 \cdot J^{-1}$	$5.7534 \cdot 10^{-3}$	$6.4875 \cdot 10^{-3}$	$6.3166 \cdot 10^{-3}$	$1.0848 \cdot 10^{-2}$	$6.4265 \cdot 10^{-3}$	$1.0369 \cdot 10^{-2}$	$8.6486 \cdot 10^{-3}$	$1.4018 \cdot 10^{-2}$
$B_8/cm^3 \cdot J^{-1}$	$2.9172 \cdot 10^{-4}$	$-8.0173 \cdot 10^{-3}$	$-1.2422 \cdot 10^{-2}$	$-1.4376 \cdot 10^{-2}$	$-1.4500 \cdot 10^{-2}$	$-1.7154 \cdot 10^{-2}$	$-1.5846 \cdot 10^{-2}$	$-7.8513 \cdot 10^{-3}$
PD/%	0.99	0.96	0.85	0.66	0.83	0.92	0.93	1.10
$\sigma/(cm^3 \cdot mol^{-1})$	0.0101	0.0108	0.0095	0.0069	0.0098	0.0110	0.0117	0.0152