Densities, Viscosities, and Refractive Indexes for Propyl Propanoate + 1-Hexanol + Benzene at 298.15 K

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Densities, cinematic viscosities, and refractive indexes of the ternary system {(x_1)propyl propanoate + (x_2)1-hexanol + (1 − x_1 − x_2)benzene} and the corresponding binary mixtures {(x_1)propyl propanoate + (x_2)1-hexanol}, {(x_1)propyl propanoate + (x_2)benzene}, and {(x_1)1-hexanol + (x_2)benzene} have been measured at 298.15 K and atmospheric pressure over the whole composition range. The excess molar volumes, dynamic viscosity deviations, and changes of the refractive index on mixing were calculated from experimental measurements. These results were fitted to a polynomial relation to estimate the coefficients and standard errors. All the experimental values were compared with the results obtained with empirical expressions that predict ternary properties from binary data.

Introduction

In previous papers,[1−5] we have reported experimental excess volumes of nonelectrolyte ternary mixtures with six carbon atoms {propyl propanoate + 1-chlorohexane + hexane},[1] {propyl propanoate + 1-chlorohexane + cyclohexane},[1] {propyl propanoate + cyclohexane + hexane},[1] {propyl propanoate + 1-hexanol + hexane},[2] {propyl propanoate + 1-hexanol + cyclohexane},[2] {propyl propanoate + 1-hexanol + 1-chlorohexane},[3] {propyl propanoate + 2-hexanone + 1-chlorohexane},[4] and {propyl propanoate + hexane + benzene}[5] at 298.15 K. In continuation of this way, we report here the excess molar volumes, dynamic viscosity deviations, and changes of refractive index on mixing of {propyl propanoate + 1-hexanol + benzene} and of the binary mixtures {propyl propanoate + 1-hexanol} and {1-hexanol + benzene} at 298.15 K. The data for the third binary mixture, {propyl propanoate + benzene}, have been published elsewhere.[5] The Cibulka equation[6] has been used to correlate the experimental values of ternary mixtures. Also, the experimental values obtained were used to test the empirical methods of Kholer,[7] Jacob and Fitzner,[8] Colinet,[1,9] Tsao and Smith,[10] Toop,[11] Scatchard et al.,[12] and Hillert.[13] These methods predict excess properties of the ternary mixtures from those of the involved binary mixtures. The results obtained for viscosities of binary mixtures were used to test the semiempirical relations of Grunberg and Nissan,[14] McAllister,[15] Ausländer,[16] and Teja and Rice.[17] The experimental refractive indexes were compared with the predicted results for the Lorentz−Lorenz, Gladstone−Dale, Wiener, Heller, and Arago−Biot equations, which were compiled by Tasic et al.[18]

Experimental Section

The chemicals employed were supplied by Fluka. Their mole-fraction purities were >0.99 for propyl propanoate, >0.99 for 1-hexanol, and >0.995 for benzene. The substances were degassed by ultrasound and dried over molecular sieves (Sigma Union Carbide, type 0.4 nm).

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Table 1. Density ρ, Dynamic Viscosity, η, and Refractive Index, n, Data for Pure Liquids at 298.15 K

	ρ/g·cm^{-3}		η/mPa·s		n	
substance	exp	lit.	exp	lit.	exp	lit.
propyl propanoate	0.875 53	0.875 52[3] 0.875 54[4]	0.641	0.6409[19]	1.3909	1.3920[19]
1-hexanol	0.815 16	0.815 19[20]	4.558	4.317[21] 4.592[22]	1.4160	1.4161[23] 1.4160[21]
benzene	0.873 45	0.873 47[24]	0.592	0.5977[25]	1.4979	1.4979[18,24]

Table 2. Densities, ρ, and Excess Molar Volumes, V_m^E, for (x)1-Hexanol + (1 − x)Benzene at 298.15 K

x	ρ/g·cm^{-3}	V_m^E/ cm^3 mol^{-1}	x	ρ/g·cm^{-3}	V_m^E/ cm^3 mol^{-1}
0.0607	0.867 40	0.1288	0.5426	0.834 69	0.3079
0.1196	0.862 28	0.2002	0.6233	0.830 75	0.2650
0.1535	0.859 51	0.2353	0.6488	0.829 58	0.2446
0.2109	0.855 10	0.2790	0.6804	0.828 13	0.2286
0.2576	0.851 73	0.3064	0.7337	0.825 78	0.1920
0.3165	0.847 74	0.3281	0.8226	0.822 04	0.1299
0.3632	0.844 78	0.3363	0.8369	0.821 46	0.1197
0.4159	0.841 59	0.3404	0.8994	0.819 01	0.0684
0.4558	0.839 30	0.3369	0.9795	0.815 94	0.0070

Excess molar volumes were determined from the densities of the pure liquids and mixtures measured with an Anton-Paar DMA 60/602 densimeter thermostated at T = (298.15 ± 0.01) K in a Haake F3 circulating-water bath. Immediately prior to each series of measurements, distilled water and heptane were used to calibrate the densimeter. The global precision obtained in the measurement of the density is better than $\pm 2 \times 10^{-6}$ g cm^{-3}. Cinematic viscosities were measured by means of a Schott−Geräte automatic viscometer with an accuracy of $\pm 5 \times 10^{-4}$ mm^2 s^{-1}. The refractive indexes were measured with a thermostated automatic refractometer Atago RX-1000, which works with the wavelength corresponding to the D line of sodium. The experimental reproducibility in the refractive index data is 1×10^{-4}. Finally, mixtures were prepared in all cases by mass using a Mettler AT 201. The precision of the mole fraction is estimated to be better than $\pm 1 \times 10^{-4}$.

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Table 3. Densities, ρ, Cinematic Viscosities, ν, and Dynamic Viscosity Deviations, $\Delta\eta$, for Binary Mixtures at 298.15 K

x	ρ/g·cm^{-3}	ν/mm^2·s^{-1}	$\Delta\eta$/mPa·s
	(x)Propyl Propanoate + (1 − x)1-Hexanol		
0.0492	0.817 99	4.6431	−0.568
0.1334	0.822 87	3.4598	−1.188
0.1938	0.826 40	2.8860	−1.413
0.2643	0.830 57	2.3646	−1.557
0.3238	0.834 10	2.0645	−1.566
0.3932	0.838 25	1.7799	−1.524
0.4490	0.841 61	1.5767	−1.470
0.5235	0.846 11	1.3568	−1.357
0.6017	0.850 85	1.1941	−1.182
0.6650	0.854 70	1.0472	−1.055
0.7365	0.859 07	0.9452	−0.858
0.7941	0.862 61	0.8741	−0.690
0.8705	0.867 35	0.8001	−0.450
0.9338	0.871 32	0.7563	−0.237
	(x)1-Hexanol + (1 − x)Benzene		
0.0654	0.866 97	0.7324	−0.223
0.1360	0.860 93	0.7875	−0.460
0.2692	0.850 94	0.9895	−0.823
0.3377	0.843 67	1.1462	−0.969
0.4240	0.841 12	1.3696	−1.126
0.4765	0.838 18	1.5522	−1.184
0.5443	0.834 63	1.8571	−1.204
0.6819	0.828 07	2.6024	−1.144
0.7508	0.825 04	3.0895	−1.023
0.8172	0.822 26	3.6813	−0.808
0.8859	0.819 53	4.3342	−0.554
0.9587	0.816 75	5.0885	−0.239

Table 4. Refractive Indexes, n, and Changes of Refractive Index on Mixing, Δn, for Binary Mixtures at 298.15 K

x	n	Δn	x	n	Δn
	(x)Propyl Propanoate + (1 − x)1-Hexanol				
0.0517	1.4145	−0.0002	0.4853	1.4028	−0.0009
0.0665	1.4140	−0.0003	0.4870	1.4029	−0.0009
0.1072	1.4129	−0.0004	0.5777	1.4006	−0.0009
0.2180	1.4099	−0.0006	0.6316	1.3992	−0.0008
0.3032	1.4076	−0.0008	0.6824	1.3980	−0.0008
0.3076	1.4074	−0.0008	0.7369	1.3968	−0.0007
0.3385	1.4066	−0.0008	0.8212	1.3948	−0.0005
0.3810	1.4055	−0.0009	0.8980	1.3931	−0.0003
0.4739	1.4031	−0.0009	0.9161	1.3926	−0.0003
	(x)1-Hexanol + (1 − x)Benzene				
0.0607	1.4901	−0.0028	0.6233	1.4387	−0.0081
0.1535	1.4793	−0.0060	0.6488	1.4369	−0.0079
0.2109	1.4735	−0.0071	0.6804	1.4349	−0.0072
0.2576	1.4688	−0.0080	0.7337	1.4314	−0.0064
0.3165	1.4630	−0.0090	0.8226	1.4260	−0.0045
0.4159	1.4545	−0.0094	0.8369	1.4251	−0.0042
0.4558	1.4512	−0.0094	0.8994	1.4214	−0.0028
0.5426	1.4445	−0.0089	0.9740	1.4174	−0.0007

Results and Discussion

The measured densities, dynamic viscosities (obtained from the measured cinematic viscosities and densities), and refractive indexes of the pure liquids are listed in Table 1 together with published values. The agreement between both sets of data indicates that the compounds used were pure and that our experimental equipment has a good accuracy. Experimental densities, dynamic viscosities, and refractive indexes for binary mixtures are listed in Tables 2−4. In previous papers[3,5] we have published the data corresponding to the binary mixtures missed in those tables.

The excess molar volumes (V_m^E), viscosity deviations ($\Delta\eta$), and changes in the refractive indexes on mixing (Δn) were computed using eqs 1−3, respectively

Table 5. Coefficients A_K and B_K of Eqs 4 and 5 and Standard Deviations, s

	A_0	A_1	A_2	A_3	A_4	A_5	s
	(x)Propyl Propanoate + (1 − x)1-Hexanol						
V_m^E [a]	0.9285	−0.0315	0.1309	0.0683			0.0007
$\Delta\eta$ [b]	−5.552	3.371	−2.918	1.638			0.008
Δn	−0.003 64	0.000 25					0.000 03
	(x)Propyl Propanoate + (1 − x)Benzene[5]						
V_m^E [a]	−0.1697	−0.0797	0.0714				0.0011
$\Delta\eta$ [b]	−0.0891	0.0540					0.0005
Δn	−0.0473	0.0115					0.0002
	(x)1-Hexanol + (1 − x)Benzene						
V_m^E [a]	1.292	−0.696	−0.116	0.513	0.403	−1.029	0.002
$\Delta\eta$ [b]	−4.770	−1.211	0.079				0.013
Δn	−0.0369	0.0103	−0.0023				0.0001
	B_1	B_2	B_3				s
	(x_1)Propyl Propanoate + (x_2)1-Hexanol + (1 − x_1 − x_2)Benzene						
$V_{m,123}^E$ [a]	0.383	7.664	−8.246				0.012
$\Delta\eta_{123}$ [b]	0.8338	2.853	5.932				0.015
Δn_{123}	0.0292	−0.0060	−0.0305				0.000 15

[a] cm^3·mol^{-1}. [b] mPa·s.

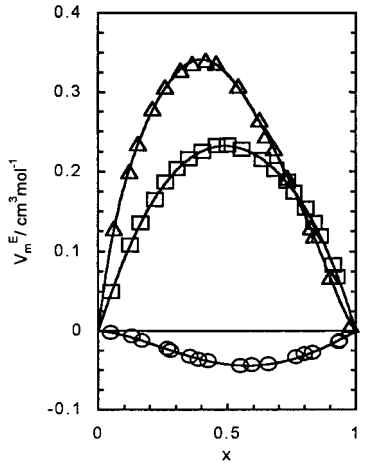

Figure 1. Excess molar volumes V_m^E at the temperature 298.15 K: ○, {(x)$C_2H_5CO_2(CH_2)_2CH_3$ + (1 − x)C_6H_6}; □, {(x)$C_2H_5CO_2$-$(CH_2)_2CH_3$ + (1 − x)$CH_3(CH_2)_5OH$}; △, {(x)$CH_3(CH_2)_5OH$ + (1 − x)C_6H_6}.

$$V_m^E = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{-1}) \quad (1)$$

$$\Delta\eta = \eta - \sum_{i=1}^{N} x_i \eta_i \quad (2)$$

$$\Delta n = n - \sum_{i=1}^{N} x_i n_i \quad (3)$$

In these equations ρ, η, and n are the density, dynamic viscosity, and refractive index in the mixture, respectively. ρ_i, η_i, and n_i are the properties of the pure components, M_i is the molar mass of component i, and N is the number of components in the mixture (so $N = 2$ in the case of a binary mixture and $N = 3$ for a ternary one). The uncertainties of the properties defined by eqs 1−3 are $\pm 2 \times 10^{-4}$ for V_m^E, $\pm 1 \times 10^{-3}$ for $\Delta\eta$, and $\pm 2 \times 10^{-4}$ for Δn. The derived excess functions of the binary systems can be represented by a Redlich−Kister type equation[26]

$$Q_{ij}^E = x_i x_j \sum_{K=0}^{m} A_K (x_i - x_j)^K \quad (4)$$

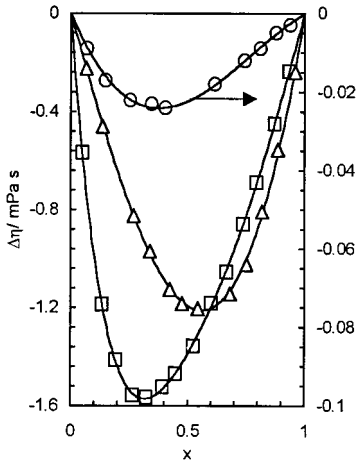

Figure 2. Experimental $\Delta\eta$ at 298.15 K: ○, {(x)$C_2H_5CO_2(CH_2)_2$-CH_3 + (1 − x)C_6H_6}; □, {(x)$C_2H_5CO_2(CH_2)_2CH_3$ + (1 − x)CH_3-$(CH_2)_5OH$}; △, {(x)$CH_3(CH_2)_5OH$ + (1 − x)C_6H_6}. Note that open dot symbols correspond to the right axis while other symbols correspond to the left axis.

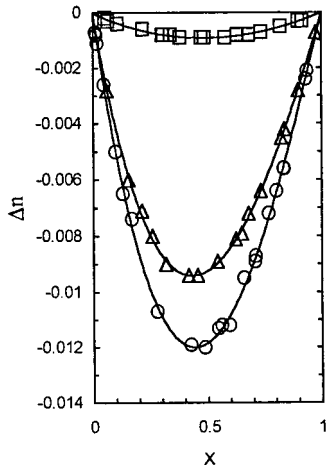

Figure 3. Experimental Δn at 298.15 K of: ○, {(x)$C_2H_5CO_2(CH_2)_2$-CH_3 + (1 − x)C_6H_6}; □, {(x)$C_2H_5CO_2(CH_2)_2CH_3$ + (1 − x)CH_3-$(CH_2)_5OH$}; △, {(x)$CH_3(CH_2)_5OH$ + (1 − x)C_6H_6}.

Table 6. Parameters for the Semiempirical Relations of Grunberg and Nissan,[14] McAllister,[15] Ausländer,[16] and Teja and Rice[17] and Standard Deviations, *s*

relation	parameters			s/mPa·s
(x)Propyl Propanoate + (1 − x)1-Hexanol				
Grunberg−Nissan	$d_w = -1.5588$			0.04
McAllister	$n_{12} = 0.8559$	$n_{21} = 1.2910$		0.02
Ausländer	$B_{12} = 1.9778$	$B_{21} = 0.1974$	$A_{21} = 0.4131$	0.013
Teja−Rice	$\alpha_{12} = -0.1399$			0.08
(x)Propyl Propanoate + (1 − x)Benzene[5]				
Grunberg−Nissan	$d_w = -0.2754$			0.016
McAllister	$n_{12} = 0.4250$	$n_{21} = 0.3706$		0.016
Ausländer	$B_{12} = 34.4216$	$B_{21} = 0.0678$	$A_{21} = 68.1872$	0.016
Teja−Rice	$\alpha_{12} = 0.7209$			0.016
(x)1-Hexanol + (1 − x)Benzene				
Grunberg−Nissan	$d_w = -0.4907$			0.08
McAllister	$n_{12} = 2.2531$	$n_{21} = 0.7915$		0.04
Ausländer	$B_{12} = 0.6730$	$B_{21} = 0.5457$	$A_{21} = 4.2753$	0.04
Teja−Rice	$\alpha_{12} = 0.5164$			0.06

where Q_{ij}^E represents any of the following properties, V_m^E, $\Delta\eta$, or Δn; x_i and x_j are the mole fractions of components i and j, respectively (note that in binary mixtures $x_i + x_j = 1$), and A_K denotes the polynomial coefficients. The degree of the polynomial Redlich−Kister equation was optimized by applying the F-test.[27] The coefficients A_K and the standard deviations, s, are given in Table 5. Figures 1−3 show the experimental V_m^E, $\Delta\eta$, and Δn plotted against x together with the fitted curves. The V_m^E is negative for the mixture propyl propanoate + benzene and positive for the other systems. The results for $\Delta\eta$ and Δn show negative curves for all the binary mixtures, while the amplitude of those excesses varies for the different mixtures.

Table 6 shows the parameters calculated and the standard deviations between experimental values obtained for dynamic viscosity and the predicted results using the semiempirical relations of Grunberg and Nissan,[14] McAllister,[15] Ausländer,[16] and Teja and Rice.[17] The values of critical temperature and critical volume for pure components were obtained from ref 22.

Table 7 compares the experimental refractive indexes for binary mixtures with the predicted results for the Lorentz−Lorenz, Gladstone−Dale, Arago−Biot, Heller, and Wiener equations, which were compiled by Tasic et al.[18]

The experimental excess molar volumes ($V_{m,123}^E$), dynamic viscosity deviations ($\Delta\eta_{123}$), and changes of refractive

Table 7. Standard Deviations of the Experimental Refractive Index Results from the Predicted for the Lorentz−Lorenz (L−L), Gladstone−Dale (G−D), Arago−Biot (A−B), Heller (H), and Wiener (W) Equations

system	L−L	G−D	A−B	H	W
(x)propyl propanoate + (1 − x)1-hexanol	0.0003	0.00014	0.0015	0.0004	0.0004
(x)propyl propanoate + (1 − x)benzene[5]	0.0029	0.0027	0.0077	0.0007	0.0011
(x)1-hexanol + (1 − x)benzene	0.0002	0.0008	0.0015	0.0014	0.0016

Table 8. Densities, ρ, and Excess Molar Volumes, $V_{m,123}^E$, at 298.15 K for the Ternary Mixture (x_1)Propyl Propanoate + (x_2)1-Hexanol + (1 − x_1 − x_2)Benzene

x_1	x_2	ρ/g·cm^{-3}	$V_{m,123}^E$/cm^3 mol^{-1}
0.0089	0.0516	0.868 31	0.1123
0.0143	0.0832	0.865 51	0.1563
0.0285	0.1655	0.858 97	0.2311
0.0431	0.2503	0.852 97	0.2777
0.0607	0.3525	0.846 63	0.2941
0.0663	0.3846	0.844 81	0.2918
0.0213	0.0458	0.868 78	0.1170
0.0608	0.1307	0.862 11	0.1849
0.0945	0.2032	0.857 13	0.2183
0.1431	0.3076	0.850 85	0.2377
0.1680	0.3612	0.847 98	0.2358
0.2151	0.4623	0.843 04	0.2216
0.0329	0.0392	0.869 64	0.0893
0.0453	0.0540	0.868 37	0.1102
0.0896	0.1070	0.864 29	0.1566
0.1355	0.1617	0.860 52	0.1920
0.1853	0.2211	0.856 98	0.2016
0.2084	0.2487	0.855 41	0.2076
0.3120	0.3724	0.849 23	0.2131
0.3819	0.4557	0.845 59	0.2144
0.0346	0.0231	0.871 21	0.0575
0.0523	0.0350	0.870 16	0.0778
0.1105	0.0740	0.867 17	0.1149
0.1722	0.1152	0.864 41	0.1369
0.4927	0.3297	0.853 19	0.2375
0.0419	0.0153	0.871 99	0.0392
0.0724	0.0264	0.871 08	0.0550
0.1397	0.0510	0.869 29	0.0772
0.0529	0.0059	0.872 92	0.0227
0.1511	0.0168	0.872 15	0.0457
0.1643	0.0183	0.872 07	0.0462
0.2601	0.0290	0.871 52	0.0539
0.3574	0.0398	0.870 98	0.0645
0.4001	0.0446	0.870 80	0.0645
0.4577	0.0510	0.870 52	0.0697
0.6016	0.0670	0.869 83	0.0902
0.7420	0.0826	0.869 17	0.1172

Table 9. Densities, ρ, Cinematic Viscosities, ν, and Dynamic Viscosity Deviations, $\Delta\eta_{123}$, at 298.15 K for the Ternary Mixture (x_1)Propyl Propanoate + (x_2)1-Hexanol + ($1 - x_1 - x_2$)Benzene

x_1	x_2	ρ/cm^3·mol^{-1}	ν/mm^2·s^{-1}	$\Delta\eta_{123}$/mPa·s
0.0815	0.8568	0.822 49	3.5943	−1.038
0.0706	0.7810	0.825 51	3.0485	−1.177
0.0773	0.6914	0.829 62	2.4688	−1.291
0.1585	0.6977	0.830 90	2.3669	−1.401
0.0690	0.6059	0.833 40	2.0509	−1.291
0.1611	0.6061	0.835 24	1.9276	−1.395
0.2506	0.5943	0.837 16	1.8093	−1.447
0.3352	0.6086	0.837 52	1.7889	−1.523
0.1584	0.5193	0.839 41	1.6079	−1.311
0.2502	0.5070	0.841 43	1.5155	−1.341
0.3421	0.5123	0.842 31	1.4911	−1.384
0.1687	0.4191	0.844 76	1.3090	−1.159
0.2469	0.4292	0.845 35	1.3135	−1.197
0.4254	0.4228	0.847 71	1.2907	−1.195
0.5180	0.4341	0.848 13	1.2828	−1.249
0.2301	0.3527	0.849 26	1.1285	−1.046
0.3322	0.3449	0.850 84	1.1036	−1.038
0.5085	0.3472	0.852 43	1.1017	−1.053
0.6000	0.3445	0.853 50	1.0734	−1.069
0.3316	0.2657	0.855 37	0.9539	−0.847
0.459	0.2581	0.856 52	0.9501	−0.823
0.5116	0.2580	0.857 30	0.9511	−0.824
0.5867	0.2469	0.858 53	0.9287	−0.801
0.6769	0.2536	0.858 97	0.9279	−0.831
0.0769	0.1685	0.859 33	0.8309	−0.555
0.1673	0.1669	0.860 37	0.8198	−0.561
0.3243	0.1672	0.861 58	0.8168	−0.570
0.4190	0.1661	0.862 26	0.8169	−0.568
0.4989	0.1672	0.862 68	0.8417	−0.554
0.5864	0.1659	0.863 29	0.8258	−0.565
0.6774	0.1567	0.864 43	0.8243	−0.532
0.7636	0.1608	0.864 79	0.8251	−0.550
0.0837	0.0843	0.866 05	0.7380	−0.297
0.1744	0.0910	0.866 19	0.7410	−0.324
0.2537	0.0818	0.867 41	0.7379	−0.292
0.4252	0.0833	0.868 13	0.7436	−0.299
0.5102	0.0831	0.868 50	0.7583	−0.288
0.5974	0.0850	0.868 71	0.7468	−0.309
0.7186	0.0640	0.870 63	0.7361	−0.238
0.7424	0.0834	0.869 41	0.7648	−0.292
0.8587	0.0801	0.870 13	0.7604	−0.287

index on mixing (Δn_{123}) for ternary mixtures were obtained using eqs 1−3, respectively. The data for these three magnitudes appear in Table 8 for $V^E_{m,123}$, in Table 9 for $\Delta\eta_{123}$, and in Table 10 for Δn_{123}. The Cibulka equation[6] has been used to correlate the experimental properties of the ternary mixtures.

$$Q^E_{123} = Q^E_{bin} + x_1x_2(1 - x_1 - x_2)(B_1 + B_2x_1 + B_3x_2) \quad (5)$$

where

$$Q^E_{bin} = Q^E_{12} + Q^E_{13} + Q^E_{23} \quad (6)$$

The symbols $Q^E_{123} = V^E_{m,123}$, $\Delta\eta_{123}$ or Δn_{123}, and Q^E_{ij} are given by eq 4 with the x_i and x_j corresponding to the ternary mixture. The parameters B_K for eq 5 and the corresponding standard deviations, s, are given in Table 5. The lines of constant ternary excess properties, calculated by eqs 5 and 6, are shown in Figures 4−6 for $V^E_{m,123}$ and $\Delta\eta_{123}$ or Δn_{123}, respectively. Figures 7−9 show lines of constant "ternary contribution", which represent the difference between the experimental value and that predicted from the binary mixtures ($Q^E_{123} - Q^E_{bin}$). Inside the triangular diagrams exist maxima and/or minima, whose coordinates are presented in Table 11.

Table 10. Refractive Indexes, n, and Changes of Refractive Index on Mixing, Δn_{123}, at 298.15 K for the Ternary Mixture (x_1)Propyl Propanoate + (x_2)1-Hexanol + ($1 - x_1 - x_2$)Benzene

x_1	x_2	n	Δn_{123}	x_1	x_2	n	Δn_{123}
0.0089	0.0516	1.4898	−0.0029	0.1105	0.0740	1.4724	−0.0076
0.0285	0.1655	1.4741	−0.0072	0.1722	0.1152	1.4603	−0.0098
0.0431	0.2503	1.4639	−0.0089	0.2378	0.1592	1.4484	−0.0110
0.0607	0.3525	1.4228	−0.0097	0.2675	0.1790	1.4435	−0.0112
0.0663	0.3846	1.4495	−0.0098	0.3106	0.2078	1.4365	−0.0111
0.0997	0.5788	1.4319	−0.0080	0.4013	0.2686	1.4237	−0.0092
0.1219	0.7075	1.4216	−0.0054	0.4927	0.3297	1.4120	−0.0061
0.0213	0.0458	1.4884	−0.0035	0.0419	0.0153	1.4891	−0.0031
0.0318	0.0684	1.4843	−0.0046	0.0724	0.0264	1.4830	−0.0050
0.0608	0.1307	1.4730	−0.0077	0.1397	0.0510	1.4706	−0.0081
0.0945	0.2032	1.4617	−0.0094	0.2098	0.0765	1.4588	−0.0103
0.1299	0.2793	1.4506	−0.0105	0.2934	0.1070	1.4465	−0.0112
0.1431	0.3076	1.4471	−0.0103	0.3326	0.1213	1.4409	−0.0115
0.1680	0.3612	1.4402	−0.0101	0.3827	0.1396	1.4343	−0.0112
0.2151	0.4623	1.4286	−0.0084	0.4977	0.1815	1.4204	−0.0093
0.2636	0.5667	1.4178	−0.0056	0.6056	0.2209	1.4089	−0.0060
0.0329	0.0392	1.4877	−0.0035	0.0529	0.0059	1.4886	−0.0031
0.0453	0.0540	1.4840	−0.0046	0.1511	0.0168	1.4729	−0.0074
0.0896	0.1070	1.4716	−0.0080	0.1643	0.0183	1.4708	−0.0080
0.1853	0.2211	1.4492	−0.0108	0.2601	0.0290	1.4574	−0.0103
0.2084	0.2487	1.4443	−0.0110	0.3574	0.0398	1.4450	−0.0114
0.2398	0.2862	1.4380	−0.0108	0.4001	0.0446	1.4398	−0.0116
0.3120	0.3724	1.4253	−0.0087	0.4577	0.0510	1.4333	−0.0114
0.3819	0.4557	1.4142	−0.0055	0.6016	0.0670	1.4185	−0.0095
0.0346	0.0231	1.4895	−0.0028	0.7420	0.0826	1.4059	−0.0058
0.0523	0.0350	1.4854	−0.0040				

Table 11. Maxima and Minima for Ternary Contributions of the Mixture (x_1)Propyl Propanoate + (x_2)1-Hexanol + ($1 - x_1 - x_2$)Benzene

	value	coordinates	
$(V^E_{m,123} - V^E_{bin})$/cm^3·mol^{-1}	max. 0.0846	$x_1 = 0.58$	$x_2 = 0.16$
	min. −0.0769	$x_1 = 0.16$	$x_2 = 0.60$
$(\Delta\eta_{123} - \Delta\eta_{bin})$/mPa·s	max. 0.148	$x_1 = 0.32$	$x_2 = 0.42$
$\Delta n_{123} - \Delta n_{bin}$	max. 0.0007	$x_1 = 0.35$	$x_2 = 0.25$

Table 12. Standard Deviations, s, of Models for (a) (x_1)Propyl Propanoate + (x_2)1-Hexanol + ($1 - x_1 - x_2$)Benzene, (b) (x_1)1-Hexanol + (x_2)Benzene + ($1 - x_1 - x_2$)Propyl Propanoate, and (c) (x_1)Benzene + (x_2)Propyl Propanoate + ($1 - x_1 - x_2$)1-Hexanol[a]

	a	b	c
	$s(V^E_{m,123})$/cm^3·mol^{-1}		
Jacob and Fitzner[8]	0.027		
Kohler[7]	0.025*		
Colinet[9]	0.026		
Tsao and Smith[10]	0.045	0.028	0.036
Toop[11]	0.027	0.029	0.026
Scatchard[12]	0.028	0.029	0.027
Hillert[13]	0.027	0.029	0.027
	$s(\Delta\eta_{123})$/mPa·s		
Jacob and Fitzner[8]	0.0891		
Kohler[7]	0.1165		
Colinet[9]	0.1094		
Tsao and Smith[10]	0.375	0.0238*	0.342
Toop[11]	0.2023	0.0252	0.136
Scatchard[12]	0.2004	0.0253	0.114
Hillert[13]	0.2004	0.0253	0.135
	$s(\Delta n_{123})$		
Jacob and Fitzner[8]	0.0004		
Kohler[7]	0.0005		
Colinet[9]	0.0004		
Tsao and Smith[10]	0.0017	0.0020	0.0002*
Toop[11]	0.0006	0.0006	0.0002*
Scatchard[12]	0.0006	0.0006	0.0002*
Hillert[13]	0.0006	0.0006	0.0002*

[a] Asterisks indicate models that give the most accurate prediction in each case.

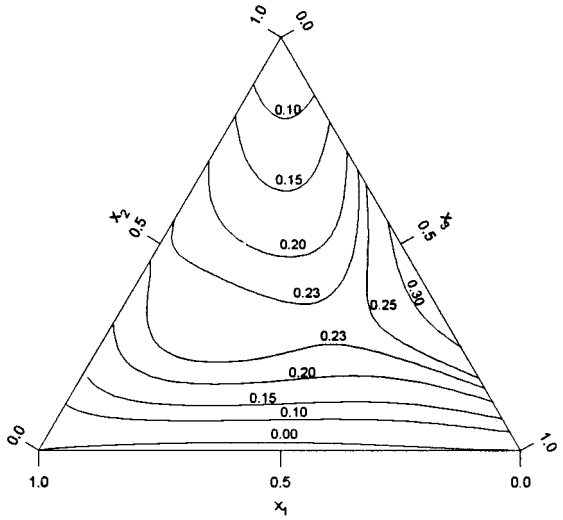

Figure 4. Curves of constant $V^{E}_{m,123}/cm^3 \cdot mol^{-1}$ for $\{(x_1)C_2H_5CO_2(CH_2)_2CH_3 + (x_2)CH_3(CH_2)_5OH + (1 - x_1 - x_2)C_6H_6\}$.

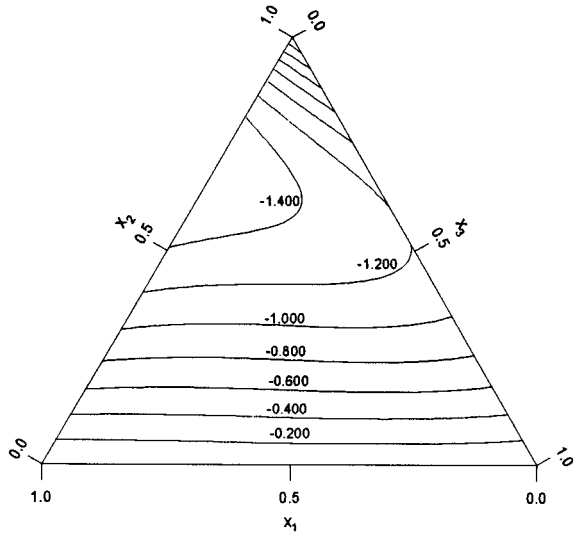

Figure 5. Curves of constant $\Delta\eta_{123}/mPa \cdot s$ for $\{(x_1)C_2H_5CO_2(CH_2)_2CH_3 + (x_2)CH_3(CH_2)_5OH + (1 - x_1 - x_2)C_6H_6\}$.

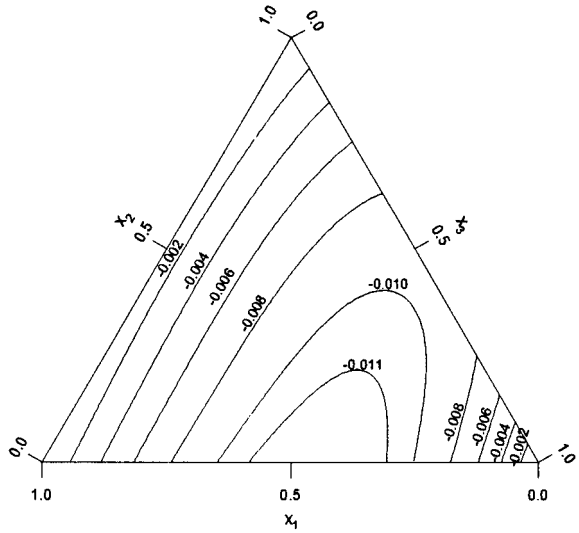

Figure 6. Curves of constant Δn_{123} for $\{(x_1)C_2H_5CO_2(CH_2)_2CH_3 + (x_2)CH_3(CH_2)_5OH + (1 - x_1 - x_2)C_6H_6\}$.

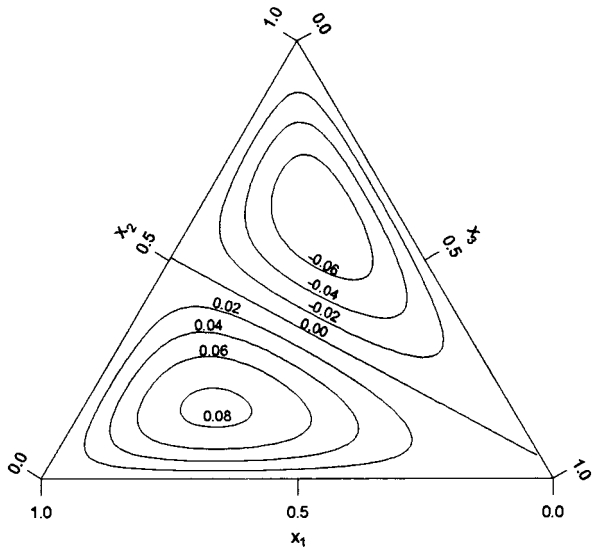

Figure 7. Curves of ternary contribution $(V^{E}_{m,123} - V^{E}_{m,bin})/cm^3 \cdot mol^{-1}$ for $\{(x_1)C_2H_5CO_2(CH_2)_2CH_3 + (x_2)CH_3(CH_2)_5OH + (1 - x_1 - x_2)C_6H_6\}$.

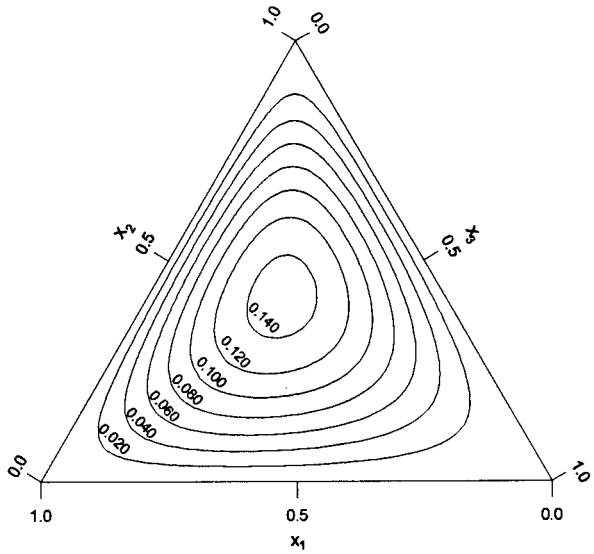

Figure 8. Curves of ternary contribution $(\Delta\eta_{123} - \Delta\eta_{bin})/mPa \cdot s$ for $\{(x_1)C_2H_5CO_2(CH_2)_2CH_3 + (x_2)CH_3(CH_2)_5OH + (1 - x_1 - x_2)C_6H_6\}$.

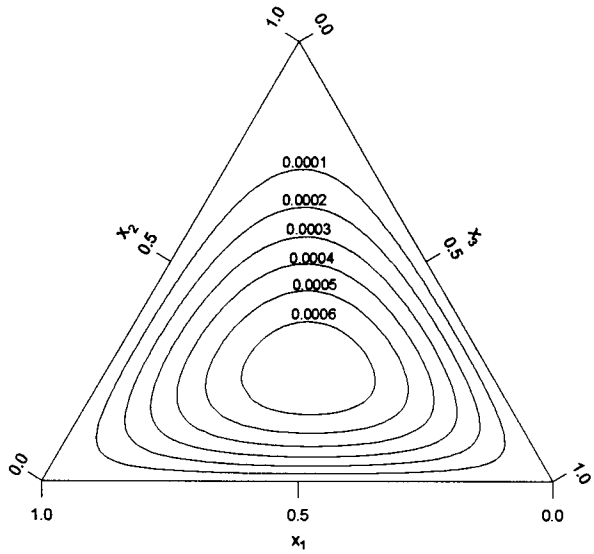

Figure 9. Curves of ternary contribution $(\Delta n_{123} - \Delta n_{bin})$ for $\{(x_1)C_2H_5CO_2(CH_2)_2CH_3 + (x_2)CH_3(CH_2)_5OH + (1 - x_1 - x_2)C_6H_6\}$.

Finally, values of $V^{E}_{m,123}$, $\Delta\eta_{123}$, and Δn_{123} have also been calculated using the empirical equations proposed by Kohler,[7] Jacob and Fitzner,[8] Colinet,[9] Tsao and Smith,[10] Toop,[11] Scatchard,[12] and Hillert,[13] which take only the binary contribution into account. For the asymmetric methods (Tsao and Smith, Toop, Scatchard, and Hillert), we must indicate the order of components in the mixtures. Table 12 shows the standard deviations between experimental and predicted values; we denote with * the most accurate predictions in each case.

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