Densities, Refractive Indices, and Excess Molar Volumes of Binary and Ternary Systems Containing Isobutyl Alcohol, Ethanol, 2-Methylpentane, and Methyl *tert*-Butyl Ether at 298.15 K

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This paper reports experimental densities and refractive indices of binary and ternary systems containing isobutyl alcohol, ethanol, 2-methylpentane, and methyl *tert*-butyl ether over the whole composition range of mixtures at 298.15 K and atmospheric pressure. From these data, excess molar volumes V^E have been calculated. These results are fitted to the Redlich−Kister and Cibulka polynomial equations to derive the binary and ternary coefficients, respectively.

Introduction

Ethers and alkanols are usually added to gasoline as oxygenates to replace lead antiknock agents, to inhibit the combustion emissions, and to reduce pollution. The commonly used oxygenating additives are methyl *tert*-butyl ether (MTBE) and light alkanols such as methanol and ethanol. Isobutyl alcohol (IBA) is added in the oxygenated gasolines with ethanol to avoid the formation of two liquid phases in the presence of small quantities of water.

In continuation of our study on mixing and excess properties for binary and ternary systems, the present work was undertaken to measure densities and refractive indices at 298.15 K for five binary mixtures (IBA + ethanol; IBA + 2-methylpentane; ethanol + 2-methylpentane; IBA + MTBE; ethanol + MTBE) and four ternary mixtures (IBA + ethanol + 2-methylpentane; IBA + ethanol + MTBE; IBA + 2-methylpentane + MTBE; ethanol + 2-methylpentane + MTBE).

Excess molar volumes were evaluated from the experimental data. This excess property for binary mixtures was fitted to the Redlich−Kister equation (1948). The binary parameters were used in the correlation of the ternary results with the Cibulka equation (1982).

Experimental Section

Chemicals. Isobutyl alcohol (99.5 mass %, HPLC grade), 2-methylpentane (99+ mass %, GC grade), and methyl *tert*-butyl ether (99.8 mass %, HPLC grade) were purchased from Aldrich. Ethanol (99.8 mass %, GC grade) was purchased from Merck. These reagents were used without further purification, after gas chromatography failed to show any significant impurities. The pure components were degassed ultrasonically and dried over molecular sieves Type 4A, $^1/_{16}$ in. The purities of the compounds were checked by determining their densities and refractive indices at 298.15 K, which were reasonably in accordance with values found in the literature (Table 1).

Apparatus and Procedure. All solutions were prepared by mass using a Mettler AE 200 balance with an accuracy of $\pm 10^{-4}$ g covering the whole composition range.

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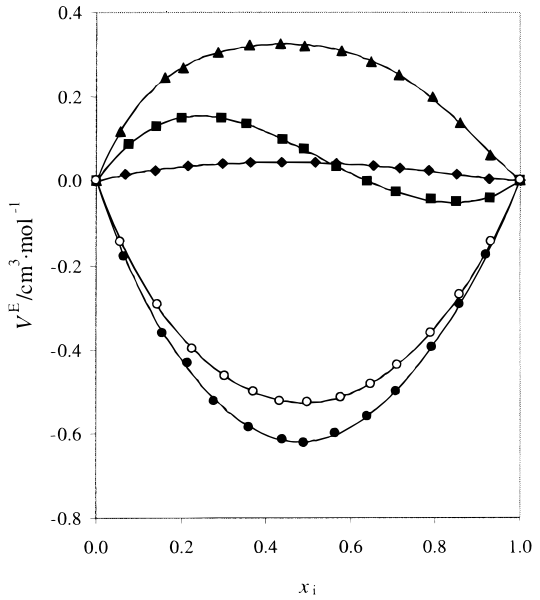

Figure 1. Excess molar volumes, V^E, as a function of composition at 298.15 K: (◆) IBA (1) + ethanol (2), $x_i = x_1$; (■) IBA (1) + 2-methylpentane (3), $x_i = x_1$; (▲) ethanol (2) + 2-methylpentane (3), $x_i = x_2$; (●) IBA (1) + MTBE (4), $x_i = x_1$; (○) ethanol (2) + MTBE (4), $x_i = x_2$; (—) Redlich−Kister equation.

Table 1. Comparison of Data with Literature Data for Pure Liquids at 298.15 K

	ρ/g·cm^{-3}		n_D	
component	this work	lit.	this work	lit.
IBA	0.797 90	0.797 93[a]	1.3938	1.3937[b]
ethanol	0.785 11	0.785 09[b]	1.3593	1.3594[c]
2-methylpentane	0.648 43	0.648 86[d]	1.3689	1.3687[c]
MTBE	0.735 29	0.735 28[c]	1.3662	1.3663[c]

[a] Sakurai et al. (1994). [b] TRC (Tables, a-6040, 1996). [c] DIPPR (Daubert and Danner, 1995). [d] Awwad and Pethtick (1983).

Precautions were taken such as using samples recently prepared and reducing to a minimum the vapor space in the vessels, to avoid preferential evaporation during manipulation and the subsequent composition errors. The possible error in the mole fraction is less than $\pm 2 \times 10^{-4}$.

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Table 2. Densities ρ, Refractive Indices n_D, and Excess Molar Volumes V^E for the Binary System at 298.15 K

x_1	ρ/g·cm^{-3}	n_D	V^E/cm^3·mol^{-1}
	IBA (1) + Ethanol (2)		
0.0682	0.786 26	1.3632	0.014
0.1378	0.787 38	1.3666	0.025
0.2151	0.788 57	1.3700	0.034
0.2966	0.789 77	1.3733	0.040
0.3624	0.790 69	1.3759	0.043
0.4356	0.791 67	1.3785	0.044
0.5143	0.792 68	1.3811	0.042
0.5678	0.793 34	1.3828	0.040
0.6537	0.794 36	1.3854	0.034
0.7171	0.795 06	1.3872	0.030
0.7835	0.795 79	1.3890	0.022
0.8491	0.796 48	1.3906	0.014
0.9270	0.797 25	1.3925	0.005
	IBA (1) + 2-Methylpentane (3)		
0.0756	0.656 07	1.3702	0.087
0.1413	0.663 18	1.3714	0.128
0.2022	0.670 12	1.3726	0.150
0.2940	0.681 30	1.3744	0.148
0.3534	0.688 96	1.3756	0.136
0.4382	0.700 57	1.3776	0.099
0.4914	0.708 22	1.3789	0.074
0.5657	0.719 46	1.3809	0.031
0.6408	0.731 39	1.3832	−0.002
0.7080	0.742 64	1.3852	−0.029
0.7904	0.757 14	1.3876	−0.046
0.8511	0.768 38	1.3896	−0.051
0.9283	0.783 37	1.3919	−0.042
	Ethanol (2) + 2-Methylpentane (3)		
0.0576	0.651 42	1.3681	0.119
0.1615	0.657 81	1.3671	0.245
0.2027	0.660 71	1.3668	0.270
0.2861	0.667 16	1.3662	0.305
0.3592	0.673 51	1.3656	0.322
0.4323	0.680 62	1.3651	0.325
0.4914	0.687 01	1.3647	0.321
0.5780	0.697 55	1.3639	0.309
0.6496	0.707 59	1.3632	0.282
0.7151	0.718 01	1.3625	0.252
0.7920	0.732 15	1.3616	0.201
0.8583	0.746 42	1.3609	0.138
0.9284	0.764 04	1.3601	0.062
	IBA (1) + MTBE (4)		
0.0658	0.739 65	1.3681	−0.179
0.1568	0.745 51	1.3708	−0.362
0.2150	0.749 10	1.3725	−0.434
0.2774	0.753 15	1.3743	−0.523
0.3609	0.758 39	1.3767	−0.587
0.4385	0.763 24	1.3789	−0.615
0.4913	0.766 56	1.3804	−0.622
0.5628	0.770 99	1.3824	−0.602
0.6392	0.775 75	1.3845	−0.560
0.7085	0.780 05	1.3864	−0.499
0.7935	0.785 32	1.3887	−0.396
0.8596	0.789 39	1.3904	−0.292
0.9204	0.793 09	1.3920	−0.177
	Ethanol (2) + MTBE (4)		
0.0578	0.737 66	1.3662	−0.145
0.1436	0.741 02	1.3662	−0.292
0.2275	0.744 37	1.3662	−0.399
0.3024	0.747 43	1.3662	−0.464
0.3706	0.750 30	1.3662	−0.501
0.4333	0.753 07	1.3661	−0.522
0.4984	0.756 05	1.3658	−0.527
0.5770	0.759 85	1.3653	−0.514
0.6477	0.763 49	1.3648	−0.484
0.7115	0.766 94	1.3642	−0.438
0.7894	0.771 42	1.3632	−0.361
0.8590	0.775 70	1.3624	−0.269
0.9333	0.780 57	1.3610	−0.146

Densities of pure components and their mixtures were measured with an Anton Paar (model DMA 55) vibrating tube densimeter. The density determination, with an accuracy of 2×10^{-5} g·cm^{-3}, is based on measuring the period of oscillation of the vibrating U-shaped sample tube filled with the sample. For each experimental set of measurements the apparatus was calibrated with doubly distilled and degassed water and dry air at atmospheric

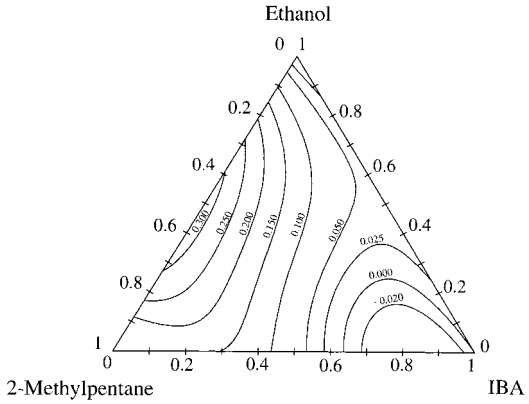

Figure 2. Curves of constant excess molar volume, V^E, for the ternary system IBA (1) + ethanol (2) + 2-methylpentane (3), at 298.15 K.

Table 3. Densities ρ, Refractive Indices n_D, and Excess Molar Volumes V^E for the Ternary System IBA (1) + Ethanol (2) + 2-Methylpentane (3) at 298.15 K

x_1	x_2	ρ/g·cm^{-3}	n_D	V^E/cm^3·mol^{-1}
0.9006	0.0460	0.786 41	1.3916	−0.029
0.7826	0.1159	0.775 49	1.3882	−0.026
0.7113	0.0891	0.756 92	1.3858	−0.032
0.7035	0.1972	0.774 46	1.3862	−0.010
0.6040	0.0902	0.737 84	1.3826	−0.020
0.6107	0.1964	0.755 52	1.3834	0.001
0.6121	0.2904	0.772 97	1.3838	0.015
0.5147	0.0908	0.722 71	1.3800	0.045
0.5030	0.2037	0.736 41	1.3800	0.036
0.5038	0.2985	0.751 82	1.3804	0.030
0.5026	0.4022	0.771 16	1.3806	0.031
0.4152	0.0900	0.707 02	1.3775	0.092
0.3992	0.2124	0.719 47	1.3770	0.083
0.4107	0.2842	0.731 67	1.3775	0.059
0.3976	0.4071	0.749 15	1.3772	0.061
0.3990	0.4991	0.767 45	1.3772	0.043
0.3071	0.1027	0.692 56	1.3748	0.145
0.3189	0.1812	0.702 68	1.3750	0.131
0.2984	0.2873	0.712 21	1.3743	0.129
0.3018	0.4026	0.729 16	1.3742	0.107
0.2935	0.5022	0.744 21	1.3734	0.091
0.3120	0.5867	0.765 38	1.3740	0.062
0.1898	0.1036	0.676 81	1.3718	0.189
0.2084	0.1845	0.686 65	1.3718	0.197
0.2122	0.2974	0.699 26	1.3716	0.186
0.2075	0.4003	0.711 29	1.3712	0.179
0.1911	0.5173	0.725 38	1.3703	0.163
0.1940	0.6120	0.742 58	1.3700	0.128
0.2047	0.6988	0.763 48	1.3700	0.086
0.1029	0.1085	0.666 31	1.3700	0.210
0.0909	0.1939	0.671 50	1.3693	0.248
0.0889	0.3157	0.682 27	1.3686	0.268
0.1034	0.4099	0.694 67	1.3684	0.252
0.0971	0.5091	0.706 11	1.3677	0.241
0.0931	0.6100	0.720 34	1.3669	0.211
0.1008	0.6949	0.737 07	1.3666	0.166
0.0922	0.8023	0.758 01	1.3655	0.106
0.0411	0.0575	0.655 79	1.3695	0.150
0.0656	0.0990	0.661 21	1.3695	0.201
0.0672	0.2015	0.669 04	1.3690	0.261
0.0565	0.3161	0.677 59	1.3678	0.286
0.0607	0.3878	0.685 36	1.3674	0.288
0.0499	0.5057	0.697 20	1.3664	0.279
0.0478	0.5966	0.709 22	1.3658	0.251
0.0440	0.7056	0.726 08	1.3646	0.211
0.0594	0.7927	0.747 14	1.3644	0.140

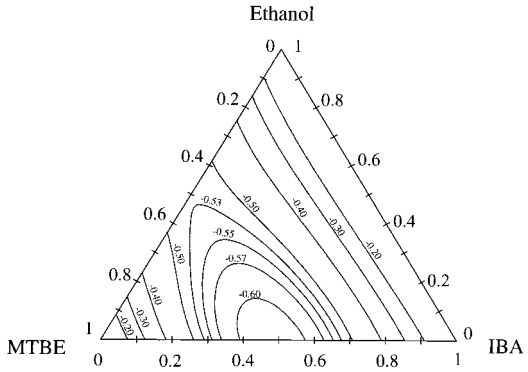

Figure 3. Curves of constant excess molar volume, V^E, for the ternary system IBA (1) + ethanol (2) + MTBE (4), at 298.15 K.

Table 4. Densities ρ, Refractive Indices n_D, and Excess Molar Volumes V^E for the Ternary System IBA (1) + Ethanol (2) + MTBE (4) at 298.15 K

x_1	x_2	ρ/g·cm^{-3}	n_D	V^E/cm^3·mol^{-1}
0.8937	0.0456	0.793 82	1.3916	−0.139
0.7814	0.1210	0.790 65	1.3887	−0.203
0.7081	0.0864	0.784 27	1.3866	−0.390
0.7093	0.1960	0.789 97	1.3868	−0.196
0.6091	0.0873	0.778 01	1.3829	−0.505
0.6006	0.2062	0.783 52	1.3839	−0.377
0.5992	0.2959	0.788 18	1.3839	−0.225
0.5154	0.0892	0.772 13	1.3816	−0.576
0.5030	0.2049	0.776 94	1.3813	−0.490
0.4947	0.3045	0.781 53	1.3811	−0.380
0.5086	0.3870	0.786 88	1.3813	−0.210
0.3998	0.0957	0.765 00	1.3783	−0.604
0.3943	0.2051	0.769 80	1.3783	−0.577
0.3875	0.3128	0.774 67	1.3782	−0.500
0.4090	0.3963	0.780 19	1.3786	−0.334
0.4019	0.5045	0.785 67	1.3781	−0.160
0.3148	0.0921	0.759 40	1.3761	−0.592
0.2942	0.2087	0.763 12	1.3751	−0.575
0.2889	0.3130	0.767 61	1.3751	−0.531
0.2990	0.4131	0.773 36	1.3752	−0.449
0.3097	0.4844	0.777 87	1.3752	−0.346
0.2997	0.6046	0.784 10	1.3742	−0.178
0.2056	0.0953	0.752 49	1.3729	−0.521
0.1891	0.2230	0.756 82	1.3726	−0.562
0.2083	0.2871	0.761 01	1.3730	−0.573
0.1969	0.3991	0.765 47	1.3725	−0.534
0.2025	0.5000	0.770 89	1.3722	−0.447
0.2095	0.5944	0.776 54	1.3720	−0.329
0.1979	0.7123	0.782 52	1.3706	−0.150
0.0893	0.1018	0.745 19	1.3698	−0.381
0.1139	0.1875	0.750 31	1.3705	−0.495
0.1067	0.2977	0.754 59	1.3702	−0.550
0.1004	0.3993	0.758 54	1.3696	−0.534
0.0914	0.5145	0.763 48	1.3688	−0.506
0.1072	0.5981	0.768 98	1.3688	−0.437
0.1023	0.6936	0.773 92	1.3678	−0.339
0.0905	0.8082	0.779 95	1.3661	−0.188
0.0615	0.0572	0.741 58	1.3686	−0.265
0.0589	0.1030	0.743 19	1.3686	−0.324
0.0575	0.1886	0.746 55	1.3687	−0.424
0.0528	0.3034	0.750 99	1.3686	−0.498
0.0480	0.4066	0.755 20	1.3682	−0.526
0.0484	0.4935	0.759 29	1.3678	−0.523
0.0453	0.5961	0.764 22	1.3672	−0.486
0.0422	0.7050	0.769 94	1.3662	−0.406
0.0566	0.8003	0.776 80	1.3655	−0.272

pressure. Temperatures were determined with a digital thermometer (Anton Paar DT 100-20). The refractive indices were measured with an Abbe refractometer (Type 3T) with an accuracy of $\pm 2 \times 10^{-4}$. Both apparatuses were connected to a Julabo circulator with proportional temperature control and an automatic drift correction system that kept the samples at the desired temperature (298.15 K) with accuracy of $\pm 10^{-2}$ K.

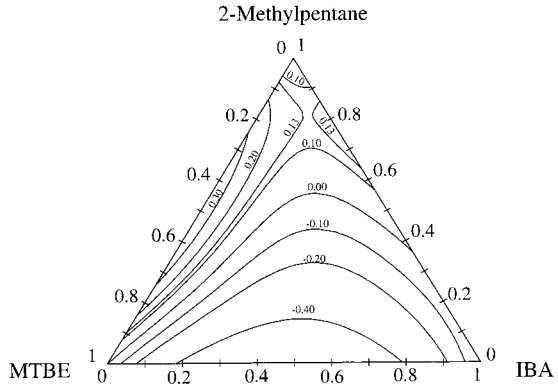

Figure 4. Curves of constant excess molar volume, V^E, for the ternary system IBA (1) + 2-methylpentane (3) + MTBE (4), at 298.15 K.

Table 5. Densities ρ, Refractive Indices n_D, and Excess Molar Volumes V^E for the Ternary System IBA (1) + 2-Methylpentane (3) + MTBE (4) at 298.15 K

x_1	x_2	ρ/g·cm^{-3}	n_D	V^E/cm^3·mol^{-1}
0.9046	0.0539	0.784 59	1.3916	−0.130
0.7992	0.0961	0.772 61	1.3886	−0.228
0.7028	0.0988	0.766 71	1.3861	−0.344
0.6974	0.1953	0.754 16	1.3854	−0.202
0.5911	0.1016	0.759 89	1.3830	−0.426
0.5985	0.1996	0.748 36	1.3829	−0.285
0.6074	0.3019	0.736 66	1.3828	−0.134
0.4908	0.1024	0.754 02	1.3802	−0.464
0.4977	0.2046	0.742 36	1.3800	−0.320
0.5044	0.2910	0.732 78	1.3800	−0.203
0.5106	0.3947	0.721 56	1.3800	−0.081
0.3887	0.1042	0.747 85	1.3775	−0.445
0.3918	0.2104	0.736 00	1.3773	−0.312
0.3963	0.2959	0.726 86	1.3773	−0.218
0.4042	0.4067	0.715 44	1.3773	−0.106
0.4047	0.5012	0.705 66	1.3773	−0.014
0.3018	0.1069	0.742 47	1.3753	−0.392
0.3069	0.1916	0.733 45	1.3752	−0.295
0.3042	0.2969	0.722 10	1.3750	−0.186
0.3121	0.3927	0.712 65	1.3752	−0.110
0.2948	0.5007	0.701 08	1.3747	−0.020
0.2950	0.6076	0.690 76	1.3748	0.054
0.1821	0.1121	0.734 85	1.3722	−0.250
0.1893	0.1993	0.726 10	1.3722	−0.166
0.1977	0.2962	0.716 72	1.3723	−0.099
0.1926	0.4031	0.705 92	1.3722	−0.016
0.1948	0.5008	0.696 75	1.3723	0.030
0.1957	0.5992	0.687 77	1.3725	0.055
0.2054	0.6997	0.679 10	1.3728	0.079
0.0982	0.0934	0.731 75	1.3698	−0.120
0.0955	0.2023	0.720 49	1.3698	−0.007
0.0955	0.2975	0.711 15	1.3698	0.066
0.0984	0.3921	0.702 33	1.3698	0.110
0.1020	0.4869	0.693 86	1.3700	0.127
0.0986	0.5953	0.684 09	1.3702	0.147
0.1020	0.6945	0.675 74	1.3706	0.133
0.1034	0.7886	0.667 94	1.3709	0.114
0.0592	0.0446	0.734 44	1.3688	−0.094
0.0615	0.0924	0.729 60	1.3688	−0.040
0.0628	0.2099	0.717 84	1.3688	0.073
0.0702	0.2938	0.710 10	1.3689	0.120
0.0662	0.3908	0.700 83	1.3690	0.170
0.0386	0.5069	0.689 03	1.3681	0.255
0.0355	0.6139	0.679 74	1.3684	0.250
0.0382	0.6969	0.673 03	1.3688	0.211
0.0324	0.8078	0.663 96	1.3690	0.154

Results and Discussion

Densities, ρ, refractive indices, n_D, and excess molar volumes, V^E, of binary and ternary mixtures are shown in Tables 2−6. In these tables, x_i is the molar fraction of component i in the mixture.

Table 6. Densities ρ, Refractive Indices n_D, and Excess Molar Volumes V^E for the Ternary System Ethanol (2) + 2-Methylpentane (3) + MTBE (4) at 298.15 K

x_1	x_2	ρ/g·cm^{-3}	n_D	V^E/cm^3·mol^{-1}
0.8990	0.0493	0.767 27	1.3618	−0.046
0.7986	0.0963	0.752 99	1.3631	−0.074
0.7047	0.1014	0.748 43	1.3646	−0.182
0.7081	0.1930	0.733 02	1.3640	0.030
0.6060	0.0966	0.745 51	1.3656	−0.272
0.5990	0.1977	0.729 74	1.3652	−0.075
0.5924	0.2965	0.715 07	1.3649	0.109
0.5011	0.1042	0.740 69	1.3664	−0.306
0.4988	0.2007	0.726 96	1.3661	−0.127
0.5123	0.2947	0.714 42	1.3656	0.033
0.4888	0.4110	0.699 16	1.3658	0.184
0.4099	0.0900	0.739 48	1.3669	−0.329
0.4054	0.1975	0.725 19	1.3666	−0.149
0.3926	0.3075	0.711 17	1.3665	0.010
0.3969	0.4085	0.699 19	1.3665	0.126
0.3923	0.5013	0.688 60	1.3665	0.205
0.2962	0.0998	0.734 44	1.3673	−0.270
0.3043	0.1933	0.723 30	1.3664	−0.135
0.3176	0.3019	0.710 78	1.3663	0.002
0.3099	0.4008	0.699 56	1.3662	0.102
0.3084	0.4931	0.689 54	1.3663	0.180
0.2873	0.6148	0.676 99	1.3654	0.256
0.1802	0.1040	0.730 31	1.3668	−0.171
0.1879	0.2076	0.718 95	1.3666	−0.045
0.1924	0.3011	0.708 99	1.3666	0.047
0.1842	0.4088	0.697 76	1.3668	0.136
0.1953	0.4921	0.689 51	1.3670	0.180
0.2009	0.6054	0.678 63	1.3670	0.208
0.2032	0.6978	0.669 85	1.3674	0.246
0.0965	0.1094	0.727 10	1.3670	−0.050
0.0955	0.1958	0.717 99	1.3670	0.049
0.0982	0.3053	0.706 96	1.3670	0.143
0.0971	0.4018	0.697 57	1.3670	0.201
0.1112	0.5082	0.687 68	1.3672	0.228
0.1012	0.5907	0.680 19	1.3674	0.243
0.1125	0.6815	0.672 19	1.3676	0.226
0.1087	0.7859	0.663 26	1.3681	0.209
0.0545	0.0449	0.732 60	1.3670	−0.059
0.0467	0.0901	0.727 55	1.3670	0.016
0.0517	0.1991	0.716 55	1.3669	0.124
0.0588	0.2923	0.707 54	1.3668	0.183
0.0504	0.3881	0.698 29	1.3670	0.251
0.0569	0.5043	0.687 76	1.3672	0.275
0.0531	0.6035	0.679 06	1.3675	0.277
0.0524	0.7045	0.670 55	1.3678	0.250
0.0515	0.7863	0.664 02	1.3682	0.185

The excess molar volumes for binary and ternary mixtures were calculated from eq 1,

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

where M_i is the molar mass of component i in the mixture,

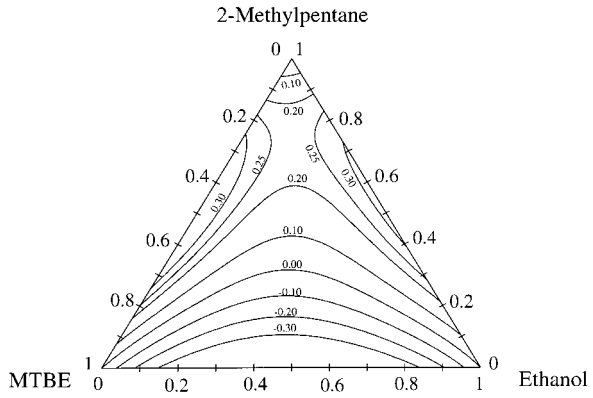

Figure 5. Curves of constant excess molar volume, V^E, for the ternary system ethanol (2) + 2-methylpentane (3) + MTBE (4), at 298.15 K.

ρ_i are the densities of the pure components, and N is the number of components in the mixture.

The V^E values for binary mixtures were correlated with the Redlich−Kister equation, according to the following expression:

$$V^E_{ij} = x_i x_j \sum_{p=0}^{m} A_p (x_j - x_i)^p \qquad (2)$$

In this equation A_p is a parameter and m is the degree of the polynomial expansion.

The excess molar volumes for the ternary mixtures were correlated using the Cibulka equation:

$$V^E_{123} = V^E_{12} + V^E_{13} + V^E_{23} + x_1 x_2 x_3 (C_1 + C_2 x_1 + C_3 x_2) \qquad (3)$$

where V^E_{12}, V^E_{13}, and V^E_{23} are the binary contributions expressed by the Redlich−Kister equation described above and C_1, C_2, and C_3 are the adjustable ternary parameters.

The unweighted least-squares method was used to fit the polynomials to the data. The parameters for fitting eqs 2 and 3 and the corresponding standard deviations obtained are given in Tables 7 and 8, respectively. The standard deviations were calculated using the following expression:

$$\sigma = \left(\frac{\sum_{i}^{n_{DAT}} (z_{exp} - z_{pred})^2}{n_{DAT} - n_{PAR}} \right)^{1/2} \qquad (4)$$

In this equation z is the value of the property, n_{DAT} is the

Table 7. Parameters of Redlich−Kister Equation and Standard Deviations σ at 298.15 K

	A_0	A_1	A_2	A_3	A_4	σ
			IBA (1) + Ethanol (2)			
V^E/cm^3·mol^{-1}	0.1724	0.0498	−0.0229	0.0425		0.0007
			IBA (1) + 2-Methylpentane (3)			
V^E/cm^3·mol^{-1}	0.2703	1.0289	0.1819	0.0341	−0.1645	0.0024
			Ethanol (2) + 2-Methylpentane (3)			
V^E/cm^3·mol^{-1}	1.2896	0.1853	0.4021	0.6475		0.0030
			IBA (1) + MTBE (4)			
V^E/cm^3·mol^{-1}	−2.4795	−0.1732	−0.0331	−0.0882	−0.2916	0.0049
			Ethanol (2) + MTBE (4)			
V^E/cm^3·mol^{-1}	−2.1118	−0.0606	−0.2580	−0.1209	−0.2755	0.0016
			2-Methylpentane (3) + MTBE (4)[a]			
V^E/cm^3·mol^{-1}	1.5915	0.0353	0.0020	−0.3961		0.0045

[a] Experimental data from Bouzas et al. (2000).

Table 8. Parameters of the Cibulka Equation and Standard Deviations σ at 298.15 K

	C_1	C_1	C_1	σ
IBA (1) + Ethanol (2) + 2-Methylpentane (3)				
V^E/cm^3·mol^{-1}	−3.2877	0.9614	1.4489	0.0053
IBA (1) + Ethanol (2) + MTBE (4)				
V^E/cm^3·mol^{-1}	1.1043	−3.2150	−1.1076	0.0087
IBA (1) + 2-Methylpentane (3) + MTBE (4)				
V^E/cm^3·mol^{-1}	−2.9908	5.1913	−5.7969	0.0174
Ethanol (2) + 2-Methylpentane (3) + MTBE (4)				
V^E/cm^3·mol^{-1}	−1.9326	3.8819	−3.5681	0.0163

number of experimental data, and n_{PAR} is the number of parameters.

Curves of excess molar volumes for binary mixtures are plotted in Figure 1. Excess molar volumes are positive for the ethanol + 2-methylpentane and IBA + ethanol systems, over the whole composition range. However, if the mixture is methyl *tert*-butyl ether + ethanol or IBA, the excess molar volumes are negative. For the binary mixture IBA + 2-methylpentane the fitted curve of excess molar volumes is sigmoidal with an initial positive region followed by a negative lobe at high IBA mole fraction.

Isolines of excess molar volumes for the ternary systems are presented in Figures 2−5. As can be expected from the behavior of binary mixtures, the ternary system IBA + ethanol + 2-methylpentane shows positive values of V^E at almost all compositions (Figure 2), except at compositions close to the binary system IBA + 2-methylpentane where a change in sign occurs. Values of V^E are negative for the whole mixtures IBA + ethanol + MTBE (Figure 3). The mixtures IBA + 2-methylpentane + MTBE (Figure 4) and ethanol + 2-methylpentane + MTBE (Figure 5) show negative and positive values of excess volumes.

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