JOURNAL OF CHEMICAL & ENGINEERING DATA

Article

pubs.acs.org/jced

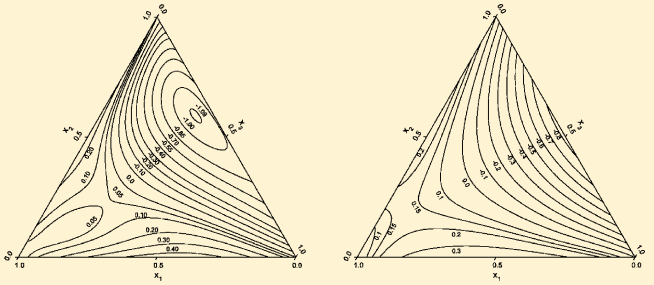
Excess Volumes of Ternary Mixtures 2,2,4-Trimethylpentane + Diisopropyl Ether or Methyl *tert*-Butyl Ether + Methanol, Ethanol, or 1-Propanol at 298.15 K

María Pilar Vela,[†] Manuela Artal,[†] José Muñoz Embid,[†] Ramón Bravo,[‡] and Santos Otín*[,†]

[†]Departamento de Química Física, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain

[‡]Departamento de Física Aplicada, Facultad de Física, Universidad de Santiago de Compostela, 15782 Santiago de Compostela, Spain

ABSTRACT: Excess volumes of six ternary mixtures formed by an alkane (2,2,4-trimethylpentane), two ethers (diisopropyl ether or methyl *tert*-butyl ether), and three alcohols (methanol, ethanol, or 1-propanol) have been determined experimentally from density measurements at the temperature of 298.15 K. Empirical equations have been fitted for the experimental results for the six ternary mixtures.



INTRODUCTION

Thermodynamic properties for pure liquids and suitably chosen binary and ternary mixtures have been studied for examining some theories of mixtures and understanding the strength and nature of the molecular interactions and for practical engineering applications. In this way, pure lower alcohols and their mixtures with branched ethers and branched alkanes have been the subject of a considerable number of investigations because they can be used to improve gasoline performance. In a previous article,[1] we have studied thermodynamic properties of binary mixtures formed by an alcohol, an ether, and an alkane. We present here the excess volumes of six ternary mixtures formed by an alkane (2,2,4-trimethylpentane), two ethers (diisopropyl ether or methyl *tert*-butyl ether), and three alcohols (methanol, ethanol, or 1-propanol), determined experimentally from density measurements at the temperature 298.15 K.

EXPERIMENTAL SECTION

Materials. The liquids used were methanol (better than 0.998 in mole fraction supplied by Fluka AG Buchs), 2,2,4-trimethylpentane, 1-propanol, methyl *tert*-butyl ether (better than 0.995 in mole fraction supplied by Fluka AG Buchs), ethanol (better than 0.995 in mole fraction supplied by Panreac S.A.), and diisopropyl ether (better than 0.999 in mole fraction supplied by Fluka AG Buchs). All the liquids were used directly without further purification. The densities of these samples are listed in Table 1 along with other literature values.

Apparatus and Procedure. Excess molar volumes of ternary mixtures were calculated at 298.15 K and atmospheric pressure from densities measurements carried out in a vibrating-tube densimeter (Anton-Paar Model DMA 60) equipped with a DMA 602 cell. The vibrating-tube temperature was measured using an Anton-Paar CKT 100 digital thermometer and was regulated to better than ±0.01 K using a Grant LT D6G thermostat. The thermometer was previously checked against the vapor pressure of benzene (better than 0.999 in mole fraction supplied by Merck) using the equation of Ambrose[3] relating temperature (T_{68}) with pressure by means of a sum of Chebyshev polynomials up to degree six (as recommended by IUPAC[4]). The densimeter calibration was performed by using doubly distilled and degassed water, benzene, and dried air. Mixtures were prepared by mass with the error in mole fraction being estimated to be less than $1\cdot10^{-4}$. Duplicate density measurements for the pure liquids agree to within $2\cdot10^{-5}$ g·cm^{-3}. Taking into account the uncertainty in the temperature, the overall total uncertainty in density is estimated to be $\leq 3\cdot10^{-5}$ g·cm^{-3}.

Table 1. Experimental Density (ρ) of Pure Liquids at T = 298.15 K

component	exptl ρ / g·cm^{-3}	lit ρ[a] / g·cm^{-3}
2,2,4-trimethylpentane	0.68762	0.68784
diisopropyl ether	0.71824	0.7182
methyl *tert*-butyl ether	0.73521	0.7353
methanol	0.78656	0.78664
ethanol	0.78531	0.78509
1-propanol	0.79970	0.79975

[a]Reference 2.

RESULTS

Experimental values of density ρ and calculated excess molar volumes of $V^{E}_{m,123}$ of the ternary mixtures are shown in Table 2.

Received: November 2, 2011
Accepted: February 20, 2012
Published: March 1, 2012

   dx.doi.org/10.1021/je2011314 | *J. Chem. Eng. Data* 2012, 57, 1139–1145

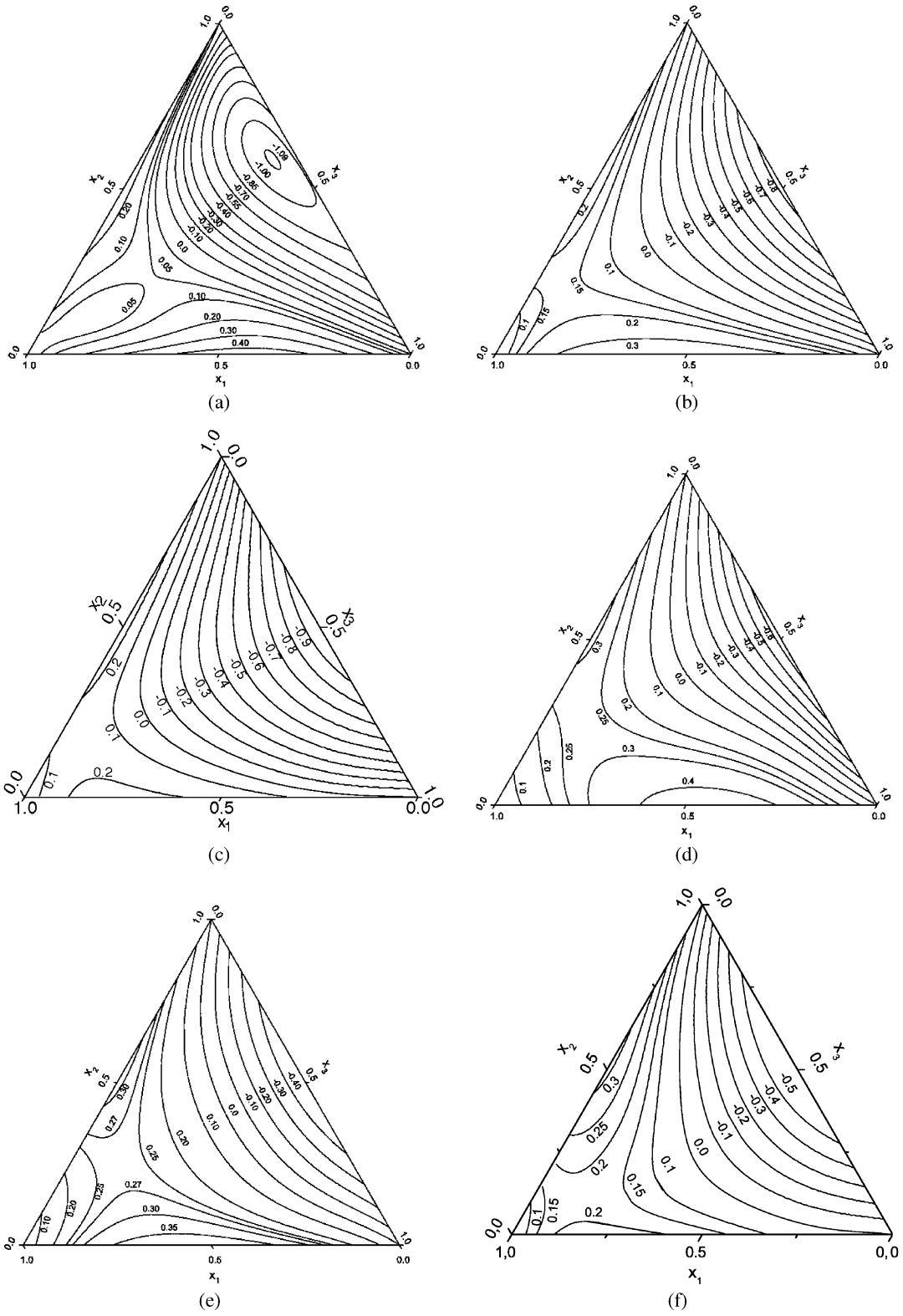


Figure 1. Curves of constant excess molar volumes $V^{E}_{m,123}$ at T = 298.15 K: 2,2,4-trimethylpentane (1) + diisopropyl ether (2) + (a) methanol (3), (b) ethanol (3), (c) 1-propanol (3); 2,2,4-trimethylpentane (1) + methyl tert-butyl ether (2) + (d) methanol (3), (e) ethanol (3), (f) 1-propanol(3).

The dependence of the experimental ternary values with the composition is expressed by the polynomial

$$V^{E}_{m,123}/(cm^3 \cdot mol^{-1}) = V^{E}_{m,12} + V^{E}_{m,13} + V^{E}_{m,23} + V^{E}_{m,ter} \quad (1)$$

where

$$V^{E}_{m,ter} = x_1x_2x_3(A_0 + A_1x_1 + A_2x_2 + A_3{x_1}^2 + A_4x_1x_2 + A_5{x_2}^2) \quad (2)$$

dx.doi.org/10.1021/je2011314 | J. Chem. Eng. Data 2012, 57, 1139–1145

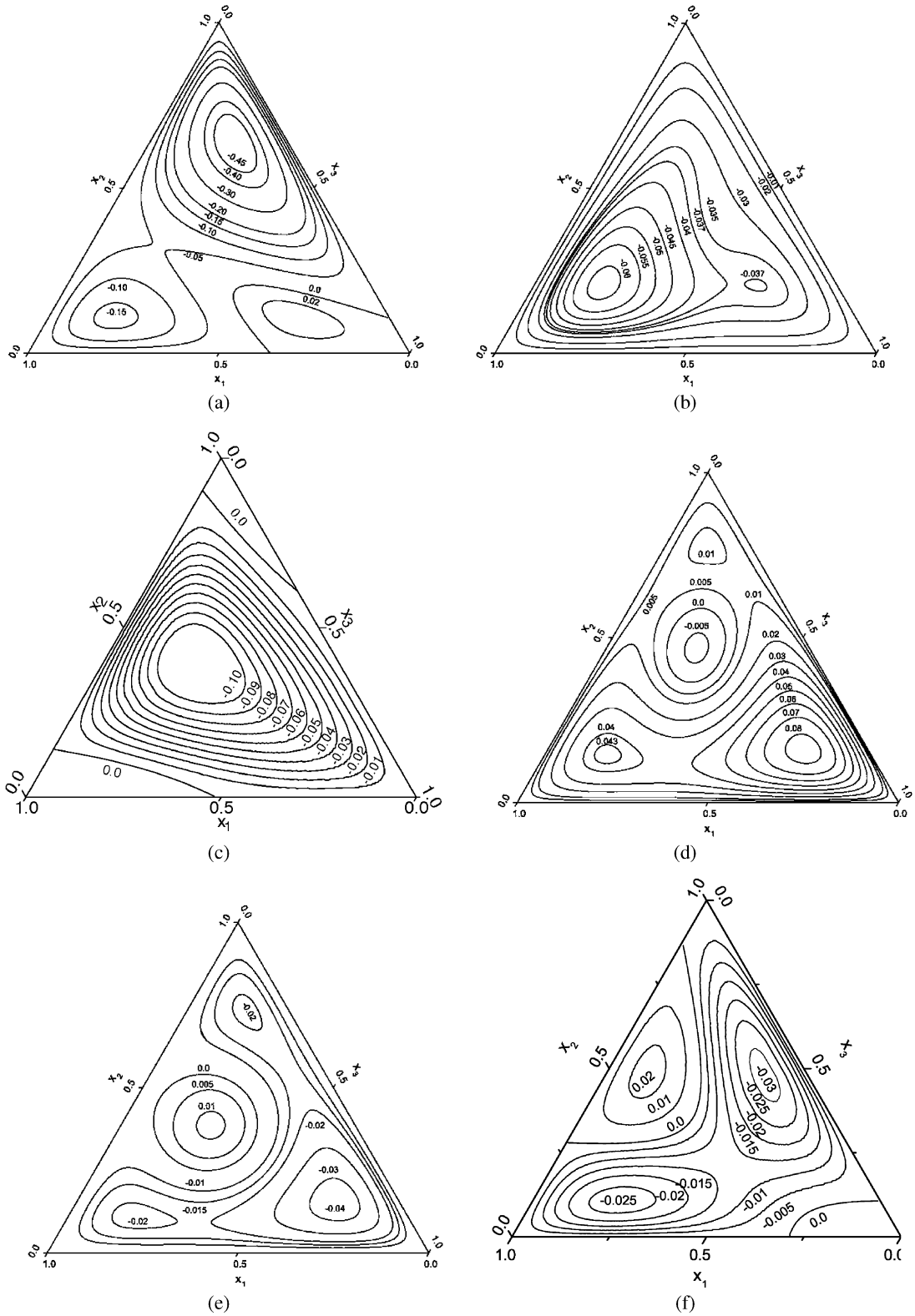


Figure 2. Ternary contribution $V^{E}_{m,ter}$ to excess molar volumes at T = 298.15 K: 2,2,4-trimethylpentane (1) + diisopropyl ether (2) + (a) methanol (3), (b) ethanol (3), (c) 1-propanol (3); 2,2,4-trimethylpentane (1) + methyl tert-butyl ether (2) + (d) methanol (3), (e) ethanol (3), (f) 1-propanol(3).

The corresponding $V^{E}_{m,12}$, $V^{E}_{m,13}$, and $V^{E}_{m,23}$ of the binary mixtures are obtained previously.[1,5−7] The bibliographic binary V^{E} data were fitted to the Redlich−Kister polynomial of eq 3 and the A_i parameters are listed in Table 3.

$$V^{E} = x_1 x_2 \sum A_i (x_1 - x_2)^{i-1} \quad (3)$$

Table 4 presents the values of the A_i parameters of eq 2 fitted to the experimental values using a nonlinear regression algorithm due to Marquardt[8] and the corresponding standard deviation. The objective function used is

$$\chi^2 = \sum [(V^{E}_{123,exp} - V^{E}_{123,cal})/(M - N)]^2 \quad (4)$$

dx.doi.org/10.1021/je2011314 | J. Chem. Eng. Data 2012, 57, 1139−1145

Table 2. Experimental Values of Density ρ and Calculated Excess Molar Volumes $V^{E}_{m,123}$ for Ternary Mixtures at the Temperature 298.15 K

x_1	x_2	ρ / g·cm^{-3}	$V^{E}_{m,123}$ / cm^3·mol^{-1}
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + Methanol (3)			
0.0354	0.0150	0.77004	0.056
0.1440	0.0610	0.73977	0.109
0.1787	0.0757	0.73357	0.109
0.2087	0.0884	0.72909	0.097
0.2496	0.1057	0.72362	0.110
0.2805	0.1188	0.72018	0.103
0.3161	0.1339	0.71672	0.092
0.3568	0.1511	0.71326	0.079
0.3931	0.1665	0.71056	0.067
0.4176	0.1768	0.70888	0.063
0.4613	0.1953	0.70612	0.064
0.4917	0.2082	0.70446	0.052
0.5244	0.2221	0.70270	0.060
0.5645	0.2391	0.70080	0.062
0.6031	0.2554	0.69909	0.072
0.6272	0.2656	0.69802	0.097
0.6649	0.2816	0.69644	0.136
0.7025	0.2975	0.69486	0.208
0.0259	0.0259	0.77238	−0.022
0.0515	0.0513	0.76157	−0.046
0.0757	0.0754	0.75335	−0.074
0.0996	0.0992	0.74666	−0.101
0.1258	0.1253	0.74053	−0.134
0.1522	0.1517	0.73527	−0.161
0.1795	0.1789	0.73052	−0.173
0.2037	0.2030	0.72696	−0.195
0.2392	0.2384	0.72232	−0.209
0.2580	0.2571	0.72016	−0.213
0.2745	0.2735	0.71841	−0.216
0.3016	0.3005	0.71575	−0.217
0.3216	0.3204	0.71394	−0.212
0.3524	0.3512	0.71135	−0.193
0.3761	0.3748	0.70943	−0.156
0.4063	0.4049	0.70723	−0.112
0.4203	0.4188	0.70625	−0.086
0.4502	0.4486	0.70416	0.001
0.4712	0.4695	0.70268	0.090
0.5009	0.4991	0.70059	0.249
0.0150	0.0342	0.77600	−0.119
0.0304	0.0690	0.76716	−0.221
0.0458	0.1041	0.75970	−0.306
0.0912	0.2072	0.74367	−0.502
0.1231	0.2797	0.73584	−0.614
0.1384	0.3146	0.73268	−0.657
0.1570	0.3568	0.72906	−0.674
0.1684	0.3826	0.72713	−0.691
0.1835	0.4171	0.72478	−0.712
0.1955	0.4443	0.72293	−0.705
0.2154	0.4894	0.72021	−0.702
0.2301	0.5229	0.71822	−0.668
0.2379	0.5407	0.71719	−0.645
0.2555	0.5807	0.71480	−0.547
0.3056	0.6944	0.70686	0.208
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + Ethanol (3)			
0.0350	0.0150	0.77411	0.003
0.0696	0.0297	0.76462	0.010
0.1045	0.0446	0.75639	0.011
0.1389	0.0593	0.74934	0.007
0.1734	0.0740	0.74304	0.012
0.2501	0.1067	0.73138	0.024
0.2868	0.1224	0.72670	0.030
0.3198	0.1365	0.72294	0.031
0.3516	0.1500	0.71958	0.038
0.3875	0.1654	0.71606	0.050
0.4181	0.1785	0.71335	0.057
0.4669	0.1993	0.70938	0.072
0.4879	0.2083	0.70777	0.083
0.5274	0.2251	0.70499	0.098
0.5620	0.2399	0.70270	0.118
0.6006	0.2563	0.70037	0.131
0.6321	0.2698	0.69860	0.143
0.6653	0.2840	0.69676	0.175
0.7009	0.2991	0.69486	0.219
0.0249	0.0246	0.77593	−0.056
0.0505	0.0500	0.76740	−0.096
0.0750	0.0742	0.76019	−0.123
0.1010	0.0999	0.75355	−0.158
0.1249	0.1235	0.74804	−0.179
0.1510	0.1494	0.74242	−0.173
0.1778	0.1759	0.73746	−0.189
0.2031	0.2009	0.73316	−0.190
0.2243	0.2219	0.72985	−0.190
0.2498	0.2471	0.72613	−0.177
0.2763	0.2733	0.72257	−0.159
0.3044	0.3011	0.71915	−0.142
0.3293	0.3258	0.71631	−0.117
0.3535	0.3497	0.71377	−0.095
0.3796	0.3755	0.71118	−0.061
0.3998	0.3955	0.70927	−0.028
0.4308	0.4262	0.70651	0.027
0.4542	0.4493	0.70449	0.090
0.4756	0.4705	0.70272	0.152
0.5027	0.4973	0.70042	0.273
0.0154	0.0353	0.77729	−0.103
0.0300	0.0687	0.77042	−0.176
0.0455	0.1041	0.76386	−0.238
0.0611	0.1399	0.75804	−0.301
0.0764	0.1750	0.75284	−0.349
0.0908	0.2080	0.74838	−0.387
0.1074	0.2461	0.74371	−0.424
0.1229	0.2816	0.73964	−0.438
0.1377	0.3155	0.73603	−0.442
0.1531	0.3507	0.73257	−0.442
0.1658	0.3799	0.72990	−0.436
0.1852	0.4243	0.72593	−0.389
0.1982	0.4540	0.72345	−0.351
0.2170	0.4970	0.72020	−0.306
0.2266	0.5190	0.71861	−0.276
0.2437	0.5582	0.71595	−0.221
0.2583	0.5917	0.71363	−0.137
0.2746	0.6289	0.71114	−0.024
0.2890	0.6621	0.70896	0.096
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + 1-Propanol (3)			
0.2451	0.1048	0.74606	−0.233
0.2793	0.1195	0.74053	−0.216

dx.doi.org/10.1021/je2011314 | J. Chem. Eng. Data 2012, 57, 1139−1145

Table 2. continued

x_1	x_2	ρ / g·cm^{-3}	$V^E_{m,123}$ / cm^3·mol^{-1}
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + 1-Propanol (3)			
0.3217	0.1376	0.73430	−0.205
0.3562	0.1524	0.72962	−0.198
0.3871	0.1656	0.72562	−0.175
0.4251	0.1819	0.72105	−0.153
0.4626	0.1979	0.71679	−0.119
0.4903	0.2097	0.71383	−0.095
0.5233	0.2238	0.71044	−0.054
0.5693	0.2435	0.70603	−0.001
0.5924	0.2534	0.70394	0.027
0.6315	0.2701	0.70054	0.082
0.6651	0.2845	0.69772	0.144
0.7004	0.2996	0.69483	0.229
0.2044	0.2007	0.74572	−0.461
0.2319	0.2277	0.74047	−0.474
0.2536	0.2489	0.73643	−0.455
0.2826	0.2775	0.73132	−0.420
0.3005	0.2950	0.72846	−0.414
0.3356	0.3294	0.72310	−0.384
0.3576	0.3510	0.71978	−0.329
0.3797	0.3728	0.71652	−0.257
0.4036	0.3962	0.71318	−0.178
0.4295	0.4216	0.70982	−0.104
0.4567	0.4483	0.70640	−0.006
0.4795	0.4707	0.70355	0.105
0.5046	0.4954	0.70041	0.262
0.1652	0.3737	0.73951	−0.635
0.1846	0.4176	0.73442	−0.607
0.2016	0.4560	0.73022	−0.569
0.2153	0.4871	0.72690	−0.519
0.2283	0.5165	0.72383	−0.454
0.2468	0.5583	0.71964	−0.349
0.2620	0.5928	0.71638	−0.259
0.2787	0.6304	0.71271	−0.100
0.2910	0.6583	0.71011	0.022
0.3066	0.6934	0.70670	0.236
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + Methanol (3)			
0.0336	0.0140	0.77121	0.089
0.0697	0.0291	0.75883	0.147
0.1063	0.0443	0.74895	0.194
0.1387	0.0578	0.74207	0.208
0.1732	0.0722	0.73584	0.226
0.2081	0.0868	0.73054	0.237
0.2475	0.1032	0.72555	0.240
0.2786	0.1162	0.72206	0.249
0.3148	0.1313	0.71852	0.253
0.3541	0.1477	0.71518	0.255
0.3869	0.1614	0.71271	0.255
0.4233	0.1766	0.71034	0.242
0.4577	0.1909	0.70821	0.245
0.4971	0.2074	0.70609	0.237
0.5298	0.2210	0.70434	0.257
0.5709	0.2382	0.70254	0.243
0.5956	0.2485	0.70140	0.263
0.6336	0.2643	0.69991	0.265
0.6652	0.2775	0.69862	0.296
0.7056	0.2944	0.69740	0.269
0.0239	0.0236	0.77432	0.025
0.0485	0.0477	0.76432	0.045
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + Methanol (3)			
0.0737	0.0726	0.75608	0.053
0.0976	0.0962	0.74963	0.054
0.1254	0.1235	0.74340	0.051
0.1511	0.1489	0.73848	0.049
0.1731	0.1706	0.73477	0.051
0.1991	0.1961	0.73094	0.053
0.2261	0.2227	0.72739	0.060
0.2531	0.2493	0.72430	0.063
0.2752	0.2711	0.72197	0.073
0.3009	0.2964	0.71963	0.072
0.3285	0.3236	0.71746	0.055
0.3487	0.3435	0.71586	0.066
0.3727	0.3672	0.71408	0.084
0.3965	0.3906	0.71241	0.109
0.4242	0.4179	0.71058	0.146
0.4550	0.4483	0.70855	0.223
0.4777	0.4706	0.70710	0.294
0.5037	0.4963	0.70572	0.340
0.0154	0.0356	0.77699	−0.047
0.0267	0.0618	0.77092	−0.069
0.0435	0.1010	0.76355	−0.119
0.0597	0.1386	0.75751	−0.152
0.0738	0.1712	0.75298	−0.177
0.0892	0.2069	0.74833	−0.172
0.1048	0.2432	0.74440	−0.184
0.1180	0.2737	0.74154	−0.201
0.1364	0.3165	0.73774	−0.195
0.1485	0.3445	0.73557	−0.196
0.1650	0.3829	0.73277	−0.185
0.1779	0.4128	0.73053	−0.140
0.1959	0.4545	0.72836	−0.169
0.2075	0.4815	0.72677	−0.144
0.2267	0.5261	0.72429	−0.090
0.2409	0.5590	0.72247	−0.026
0.2566	0.5953	0.72088	0.002
0.2729	0.6333	0.71898	0.096
0.2876	0.6674	0.71719	0.218
0.3012	0.6988	0.71586	0.291
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + Ethanol (3)			
0.0361	0.0145	0.77452	0.016
0.0698	0.0280	0.76561	0.047
0.1054	0.0423	0.75756	0.066
0.1423	0.0572	0.75022	0.087
0.1754	0.0705	0.74457	0.087
0.2196	0.0882	0.73763	0.117
0.2503	0.1006	0.73345	0.124
0.2878	0.1156	0.72877	0.137
0.3189	0.1281	0.72538	0.131
0.3558	0.1430	0.72147	0.155
0.3901	0.1567	0.71814	0.180
0.4317	0.1734	0.71443	0.212
0.4660	0.1872	0.71167	0.231
0.5009	0.2013	0.70913	0.240
0.5316	0.2136	0.70705	0.248
0.5705	0.2292	0.70458	0.259
0.6067	0.2438	0.70250	0.260
0.6531	0.2624	0.70001	0.265
0.6757	0.2715	0.69886	0.272

dx.doi.org/10.1021/je2011314 | *J. Chem. Eng. Data* 2012, 57, 1139–1145

Table 2. continued

x_1	x_2	ρ / g·cm^{-3}	$V^E_{m,123}$ / cm^3·mol^{-1}
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + Ethanol (3)			
0.7134	0.2866	0.69717	0.251
0.0242	0.0240	0.77686	−0.009
0.0495	0.0491	0.76910	−0.016
0.0739	0.0733	0.76256	−0.029
0.1003	0.0995	0.75621	−0.036
0.1254	0.1245	0.75077	−0.036
0.1441	0.1430	0.74704	−0.032
0.1723	0.1710	0.74190	−0.025
0.2020	0.2005	0.73690	0.003
0.2246	0.2229	0.73351	0.017
0.2519	0.2500	0.72979	0.027
0.2788	0.2768	0.72641	0.042
0.3061	0.3038	0.72316	0.075
0.3284	0.3260	0.72076	0.091
0.3526	0.3500	0.71830	0.114
0.3779	0.3751	0.71590	0.138
0.4060	0.4030	0.71339	0.171
0.4244	0.4213	0.71183	0.196
0.4446	0.4413	0.71018	0.227
0.4780	0.4745	0.70752	0.300
0.5019	0.4981	0.70590	0.321
0.0139	0.0324	0.77933	−0.061
0.0297	0.0695	0.77296	−0.107
0.0432	0.1009	0.76814	−0.148
0.0588	0.1374	0.76283	−0.170
0.0740	0.1728	0.75816	−0.189
0.0910	0.2126	0.75324	−0.187
0.1048	0.2450	0.74982	−0.211
0.1189	0.2779	0.74637	−0.208
0.1348	0.3151	0.74279	−0.202
0.1517	0.3545	0.73926	−0.188
0.1665	0.3891	0.73634	−0.169
0.1785	0.4171	0.73416	−0.156
0.1924	0.4495	0.73171	−0.128
0.2100	0.4906	0.72876	−0.086
0.2240	0.5233	0.72643	−0.028
0.2404	0.5617	0.72398	0.023
0.2511	0.5867	0.72245	0.058
0.2683	0.6270	0.72006	0.130
0.2867	0.6698	0.71755	0.230
0.2997	0.7003	0.71600	0.280
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + 1-Propanol (3)			
0.2002	0.0983	0.75466	−0.111
0.2366	0.1161	0.74842	−0.106
0.2692	0.1321	0.74322	−0.096
0.3033	0.1489	0.73818	−0.093
0.3420	0.1679	0.73257	−0.040
0.3716	0.1824	0.72868	−0.017
0.4049	0.1987	0.72462	0.000
0.4404	0.2162	0.72049	0.029
0.4677	0.2296	0.71745	0.059
0.5069	0.2488	0.71336	0.097
0.5375	0.2638	0.71035	0.129
0.5717	0.2806	0.70710	0.175
0.6060	0.2975	0.70399	0.227
0.6707	0.3293	0.69867	0.284
0.1228	0.1219	0.76610	−0.189
0.1506	0.1495	0.75983	−0.199
0.1739	0.1726	0.75490	−0.200
0.2000	0.1985	0.74978	−0.207
0.2281	0.2265	0.74459	−0.207
0.2503	0.2485	0.74063	−0.190
0.2783	0.2763	0.73588	−0.159
0.3029	0.3007	0.73182	−0.109
0.3282	0.3259	0.72801	−0.078
0.3487	0.3462	0.72503	−0.043
0.3776	0.3749	0.72102	0.009
0.3989	0.3960	0.71816	0.060
0.4226	0.4196	0.71512	0.116
0.4467	0.4435	0.71212	0.184
0.4749	0.4715	0.70874	0.278
0.5018	0.4982	0.70583	0.336
0.0892	0.2078	0.76721	−0.341
0.1072	0.2496	0.76171	−0.361
0.1206	0.2808	0.75783	−0.375
0.1386	0.3228	0.75286	−0.385
0.1520	0.3539	0.74924	−0.370
0.1645	0.3832	0.74596	−0.350
0.1795	0.4182	0.74220	−0.323
0.1980	0.4612	0.73765	−0.260
0.2091	0.4869	0.73509	−0.225
0.2257	0.5256	0.73133	−0.159
0.2378	0.5537	0.72873	−0.112
0.2556	0.5952	0.72494	−0.019
0.2709	0.6310	0.72173	0.081
0.3004	0.6996	0.71584	0.294

where M is the number of experimental data points, and N is the number of fitted parameters. Curves of constant $V^E_{m,123}$ have been plotted in Figure 1 for the six ternary studied systems, and Figure 2 shows the ternary contributions $V^E_{m,ter}$ given by eq 2 to excess molar volumes.

DISCUSSION

As far as we know, the only previous studies on these type of mixtures are those for ternary 2,2,4-trimethylpentane + diisopropyl ether + ethanol[9,10] at (298.15 and 303.15) K and 2,2,4-trimethylpentane + diisopropyl ether +1-propanol[11] at 303.15 K. Their results show a good concordance with ours.

Excess volumes of the binary mixtures of alcohol or ether + alkane previously studied[1,5−7] are positive and increase with increasing length in the aliphatic chain of alcohol and ether. For alcohol + ether, $V^E_{m,123}$ values are negative showing that the geometrical and interactional effects should be important in these mixtures, taking into account that their H^Es are positive.[12]

The addition of alcohol to binary mixtures alkane + ether decreases the volume $V^E_{m,123}$. This effect is more pronounced in the ether-rich region. As the aliphatic chain of the alcohol gets longer, the extent of the contraction increases both in the 2,2,4-trimethylpentane + diisopropyl ether and the 2,2,4-trimethylpentane + methyl *tert*-butyl ether mixtures. The experimental excess volumes point to the importance not only of the

dx.doi.org/10.1021/je2011314 | J. Chem. Eng. Data 2012, 57, 1139−1145

Table 3. Parameters A_i of eq 3 for the Bibliographic V^E Data

	A_0	A_1	A_2	A_3	A_4
2,2,4-trimethylpentane (1)					
+ diisopropyl ether (2)	1.0300	−0.0892	−0.1282		
+ methyl *tert*-butyl ether (2)	1.2534	−0.1693			
+ methanol (2)	1.7994	−0.4664	0.1924		
+ ethanol (2)	1.5882	0.1521	0.5588	0.3892	0.7371
+ 1-propanol (2)	0.6947	0.6697	−0.0064	0.8300	1.1501
diisopropyl ether (1)					
+ methanol (2)	−3.9457	−0.2849	−0.8878	−0.1560	
+ ethanol (2)	−3.3279	−0.2941	−0.7760		
+ 1-propanol (2)	−3.9770	−0.1415	−0.8844		
methyl *tert*-butyl ether (1)					
+ methanol (2)	−2.5943	−0.1183	−0.3788		
+ ethanol (2)	−2.0168	−0.1003	−0.1484	−0.1724	
+ 1-propanol (2)	−2.5410	−0.2170	−0.6450	−0.6960	

Table 4. Parameters A_i of eq 2 and Standard Deviations s

						s
A_0	A_1	A_2	A_3	A_4	A_5	$cm^3 \cdot mol^{-1}$
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + Methanol (3)						
4.0862	7.363	−34.292	−50.809	116.02	−43.125	0.020
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + Ethanol (3)						
−5.4269	15.840	13.044	−18.782	−16.716	−11.896	0.009
2,2,4-Trimethylpentane (1) + Diisopropyl Ether (2) + 1-Propanol (3)						
−4.2300	7.774	6.787	0.897	−33.603	0.277	0.012
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + Methanol (3)						
14.425	−38.293	−37.827	32.647	40.262	27.342	0.021
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + Ethanol (3)						
−7.8464	20.159	21.591	−17.571	−16.532	−19.224	0.016
2,2,4-Trimethylpentane (1) + Methyl *tert*-Butyl Ether (2) + 1-Propanol (3)						
1.1851	−3.024	−12.058	−3.7883	27.9728	8.840	0.010

intermolecular effects (self-association in the alcohol, dipole−dipole interactions between monomers and multimers, dispersion forces, etc.) but also of the free volume effects in the ternary mixtures.

AUTHOR INFORMATION

Corresponding Author

*E-mail: santos@unizar.es.

Funding

We gratefully acknowledge financial support received from the Spanish MICINN-FEDER (Project CTQ2008-02037) and Convenio Gobierno de Aragón, Obra Social "La Caixa" 2009.

Notes

The authors declare no competing financial interest.

REFERENCES

(1) Blanco, S. T.; Muñoz Embid, J.; Otín, S. Excess Volumes of (2,2,4-Trimethylpentane + Methanol or Ethanol or Propan-2-ol or Di-1-methylethyl Ether or 1,1-Dimethylethyl Methyl Ether) and of (Methanol or Ethanol or Propan-2-ol + Di-1-methylethyl ether or 1,1-Dimethylethyl Methyl Ether) at the Temperature 298.15 K. *J. Chem. Thermodyn.* **1994**, *26*, 23−28.

(2) *TRC Thermodynamic Tables*; Thermodynamics Research Center, Texas A&M University: College Station, TX, 1963/1966/1990.

(3) Ambrose, D. Recommended Reference Materials for the Realization of Physicochemical Properties. *Pure Appl. Chem.* **1977**, *49*, 1437−1464.

(4) Marsh, K. N. *Recommended Reference Materials for the Realization of Physicochemical Properties*; Blackwell Scientific Publications: Oxford, U.K., 1987.

(5) Kammerer, K.; Lichtenthaler, R. N. Excess Properties of Binary Alkanol-Ether Mixtures and the Application of the ERAS Model. *Thermochim. Acta* **1998**, *310*, 61−67.

(6) Pal, A.; Dass, G. Excess Molar Volumes and Viscosities for Binary Liquid Mixtures of Methyl tert-Butyl Ether and of tert-Amyl Methyl Ether with Methanol, 1-Propanol, and 1-Pentanol at 298.15 K. *J. Chem. Eng. Data* **1999**, *44*, 1325−1329.

(7) Berro, C. Excess Volumes, Liquid-Vapor Equilibrium, and Excess Gibbs Energy of Some Binary Mixtures Containing Alkanols (1-Propanol, 2-Propanol, 2-Methyl-1-propanol) and Normal Alkanes (C_6-C_9) or 2,2,4-Trimethylpentane. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1987**, *2*, 85−104.

(8) Marquardt, D. W. An Algorithm for Least-Squares Estimation of Nonlinear Parameters. *J. Soc. Ind. Appl. Math.* **1963**, *11*, 431−441.

(9) Chen, H. W.; Tu, C. H. Densities, Viscosities, and Refractive Indices for Binary and Ternary Mixtures of Diisopropyl Ether, Ethanol, and 2,2,4-Trimethylpentane. *J. Chem. Eng. Data* **2006**, *51*, 261−267.

(10) Kim, H. D.; Hwang, I. C.; Park, S. J. Isothermal Vapor-Liquid Equilibrium at 333.15 K and Excess Molar Volumes, Refractive Indices, and Excess Molar Enthalpies at 303.15 K for the Binary and Ternary Mixtures of Di-isopropyl Ether, Ethanol, and 2,2,4-Trimethylpentane. *J. Chem. Eng. Data* **2009**, *54*, 3051−3058.

(11) Hwang, I. C.; Jo, M. Y.; Kwak, H. Y.; Park, S. J.; Han, K. J. Isothermal VLE and V^E at 303.15 K for the Binary and Ternary Mixtures of Di-isopropyl Ether (DIPE) + 1-Propanol + 2,2,4-Trimethylpentane. *J. Chem. Eng. Data* **2007**, *52*, 2503−2508.

(12) Villamañan, M. A.; Casanova, C.; Roux, A.; Grolier, J.-P. Calorimetric Investigation of the Interactions between Oxygen and Hydroxil Groups in (Alcohol + Ether) at 298.15 K. *J. Chem. Thermodyn.* **1982**, *14*, 251−258.