Isothermal Vapor–Liquid Equilibrium of Ternary Mixtures Containing 2-Methyl-1-propanol or 2-Methyl-2-propanol, n-Hexane, and 1-Chlorobutane at 298.15 K

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Isothermal Vapor−Liquid Equilibrium of Ternary Mixtures Containing 2-Methyl-1-propanol or 2-Methyl-2-propanol, *n*-Hexane, and 1-Chlorobutane at 298.15 K

Hernando Guerrero, Ignacio Giner, Héctor Artigas, Carlos Lafuente, and Ignacio Gascón*

Departamento de Química Orgánica-Química Física, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain

Isothermal vapor−liquid equilibrium for the ternary mixtures 2-methyl-1-propanol + *n*-hexane + 1-chlorobutane and 2-methyl-2-propanol + *n*-hexane + 1-chlorobutane and for the binary mixtures 2-methyl-1-propanol + *n*-hexane and 2-methyl-2-propanol + *n*-hexane have been studied at *T* = 298.15 K. The experimental data were checked for thermodynamic consistency using the method of van Ness. The isothermal vapor−liquid equilibrium data of the ternary mixtures together with the corresponding constituent binary mixtures were correlated with the Wilson equation. The G^E values obtained have been compared with those of the ternary mixtures 1-butanol or 2- butanol + *n*-hexane + 1-chlorobutane previously investigated.

1. Introduction

The study of vapor−liquid equilibrium (VLE) of multicomponent liquid mixtures in isothermal conditions provides experimental data of great interest in thermodynamics and chemical engineering and contributes decisively for the development of accurate methods to predict and correlate phase equilibrium. However, relatively few investigations on isothermal VLE of ternary mixtures can be found in the literature.

In the past years, our laboratory has been involved in the study of several thermodynamic and transport properties of the ternary mixtures containing an isomer of butanol + *n*-hexane + 1-chlorobutane,[1−7] and we also have recently reported isothermal VLE data for the ternary systems 1-butanol or 2-butanol + *n*-hexane + 1-chlorobutane at 298.15 K.[8] To complete this systematic study, we report here vapor−liquid equilibrium data obtained at 298.15 K for the ternary systems 2-methyl-1-propanol or 2-methyl-2-propanol + *n*-hexane + 1-chlorobutane and for the binary mixtures 2-methyl-1-propanol or 2-methyl-2-propanol + *n*-hexane. Thermodynamic consistency of the experimental data has been checked by the method of van Ness.[9] We have also correlated activity coefficients of the components and excess Gibbs function of the mixtures using the Wilson equation.[10]

To the best of our knowledge, there is not any isothermal VLE study on the ternary systems presented here, although there are some previous reports on the constituent binary systems at different temperatures: 2-methyl-1-propanol + *n*-hexane,[11,12] 2-methyl-2-propanol + *n*-hexane,[12,13] 2-methyl-1-propanol + 1-chlorobutane,[14] 2-methyl-2-propanol + 1-chlorobutane,[15] and *n*-hexane + 1-chlorobutane.[16,17]

2. Experimental Section

To obtain the isothermal vapor−liquid equilibrium of the systems studied, the compounds 2-methyl-1-propanol (purity better than 99.5 % in mass fraction), 2-methyl-2-propanol, *n*-hexane, and 1-chlorobutane (better than 99 % in mass fraction) were obtained from Aldrich. The alcohols were stored under

activated molecular sieves of type 0.3 nm from Merck. The purity of the chemicals was checked by comparing experimental densities and vapor pressures at the temperature of 298.15 K with those reported in the literature.[11,12,14,15,18,19] No further purification was considered necessary. Densities were measured with a density and sound analyzer (Anton Paar DSA-5000), while vapor pressures were determined using the same apparatus employed in the VLE study. Both properties, together with literature values, are collected in Table 1, and the agreement between experimental and literature values can be considered satisfactory. In this table, we also have included the measured speeds of sound of the pure compounds.

The vapor−liquid equilibrium was studied using an all-glass dynamic recirculating type still, which was equipped with a Cottrell pump. This is a commercial unit (Labodest model) built in Germany by Fischer. The equilibrium temperatures were measured by means of a thermometer (model F25 with a PT100 probe) from Automatic Systems Laboratories, and the pressure was measured with a Digiquartz 735-215A-102 pressure transducer from Paroscientific equipped with a Digiquartz 735 display unit. The pressure in the still can be modified to obtain the desired boiling temperature by means of a vacuum pump and dry air. The total volume of liquid in the still is 150 mL, and the steady state corresponding to equilibrium is usually attained after 30 min of recirculation. The uncertainty in measurement of the pressure and temperature equilibrium in the still is ± 5 Pa and ± 0.01 K, respectively. The compositions of both liquid- and vapor-condensed phases have been analyzed by measuring their density and speed of sound with a density and sound analyzer (Anton Paar DSA-5000) calibrated with deionized doubly distilled water and dry air. The uncertainty of the density measurements is ± 0.001 kg·m^{-3}, and the corresponding uncertainty for speed of sound measurements is ± 0.01 m·s^{-1}. Density and speed of sound composition dependence for the ternary mixtures were previously determined using the same apparatus (density and speed of sound measurements for the ternary mixtures can be found in the Supporting Information). Experimental uncertainty in liquid and vapor mole fractions can be estimated in ± 0.0002 for binary mixtures and ± 0.001 for ternary mixtures.

* Corresponding author. Tel.: +34 976761200. Fax: + 34 976761202. E-mail address: igascon@unizar.es.

Table 1. Properties of the Pure Compounds at 298.15 K and Comparison with Literature Data

compound	p^{exp} (Pa)	p^{lit} (Pa)	ρ^{exp} (kg·m^{-3})	ρ^{lit} (kg·m^{-3})	u (m·s^{-1})	$B \cdot 10^6$ (m^3·mol^{-1})
2-methyl-1-propanol	1535	1501[a]	797.775	797.94[d]	1187.95	−5009
2-methyl-2-propanol	5605	5610[b]	780.885	780.63[e]	1121.50	−4390
n-hexane	20220	20174[c]	654.960	654.88[d]	1078.05	−1919
1-chlorobutane	13515	13499[b]	880.805	880.75[f]	1118.15	−1722

[a] From ref 14. [b] From ref 15. [c] From ref 12. [d] From ref 11. [e] From ref 18. [f] From ref 19.
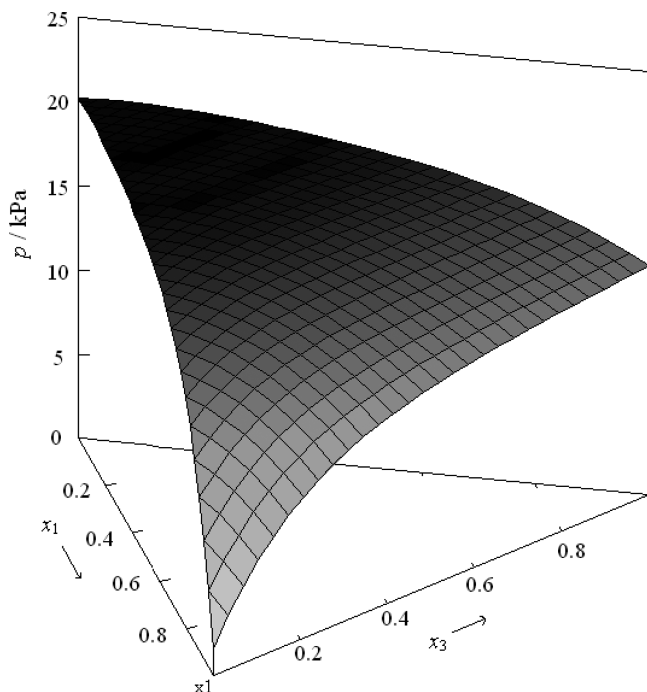
Figure 1. Vapor pressure−liquid composition surface calculated with the Wilson equation for the ternary system 2-methyl-1-propanol (1) + n-hexane (2) + 1-chlorobutane (3) at 298.15 K.

The proper operation of the different devices was periodically checked and calibrated if necessary.

3. Results and Discussion

The vapor−liquid equilibrium data at 298.15 K, p, x_1, x_2, y_1, and y_2, together with the correlated activity coefficients and excess Gibbs functions, are given in Table 2.

The Wilson equation has been used to correlate the activity coefficients of the components in the liquid phase

$$\ln \gamma_i = -\ln\left(\sum_{j=1}^{N} x_j \Lambda_{ij}\right) + 1 - \sum_{k=1}^{N} \frac{x_k \Lambda_{ki}}{\sum_{j=1}^{N} x_j \Lambda_{kj}} \quad (1)$$

$$\Lambda_{ij} = \frac{V_j^o}{V_i^o} \exp\left(-\frac{\lambda_{ij} - \lambda_{ii}}{RT}\right) \quad \Lambda_{ii} = \Lambda_{jj} = 1 \quad \lambda_j = \lambda_{ji} \quad (2)$$

where γ_i are the activity coefficients of the components; x_j and x_k are, respectively, the mole fractions of components j and k in the liquid phase; $(\lambda_{ij} - \lambda_{ij})$ are the Wilson parameters; V_i^o is the molar volume of component i in the liquid phase; R is the gas constant; and T is the temperature.

In this correlation, we have considered simultaneously isothermal VLE data at 298.15 K reported here for the binary (butanol + n-hexane) and ternary (butanol + n-hexane + 1-chlorobutane) mixtures together with the other constituent

binary mixtures (butanol + 1-chlorobutane and n-hexane + 1-chlorobutane) which were taken from the literature.[14,15,17] VLE data for the binary mixtures butanol + 1-chlorobutane[14,15] were measured using a static method, thus vapor compositions have not been reported in the literature. Consequently, for these binary data only the average pressure deviation has been calculated but not the average vapor composition deviation.

Estimation of the adjustable parameters of the Wilson equation was based on minimization of the following objective function in terms of experimental and calculated pressure values[20]

$$F = \sum_{i=1}^{n} \left(\frac{p^{exp} - p^{cal}}{p^{exp}}\right)^2 \quad (3)$$

n being the number of experimental points.

The calculated pressure is obtained taking into account both the nonideality of the vapor phase and the variation of the Gibbs function of the pure compounds with pressure as follows

$$p^{cal} = \sum_{i=1}^{3} x_i \gamma_i p_i^o \exp\left[\frac{(V_i^o - B_{ii})(p - p_i^o)}{RT} - \right.$$

$$\left. \frac{p}{2RT} \sum_j \sum_k y_j y_k (2\delta_{ji} - \delta_{jk})\right] \quad (4)$$

$$\delta_{ji} = 2B_{ji} - B_{jj} - B_{ii} \quad (5)$$

where x_i and y_i are, respectively, the mole fractions of component i in the liquid phase and in the vapor phase; p is the total pressure; p_i^o are the vapor pressures of the pure compounds; B_{ii} are the second virial coefficients that were taken from TRC-Tables;[21] and B_{ij} is the cross second virial coefficient calculated using a suitable mixing rule,[22] $B_{ij} = (1/8)(B_{ii}^{1/3} + B_{jj}^{1/3})^3$. Values of second virial coefficients of pure compounds are collected in Table 1.

The Wilson parameters for the activity coefficient correlation along with average deviations in pressure, Δp, for the whole correlated data (ternary system + binary constituent systems) are gathered in Table 3. The average deviations for pressure are (106 and 89) Pa, respectively.

The thermodynamic consistency of the VLE data was also checked for the binary and ternary mixtures simultaneously using the van Ness method[9] described by Fredenslund et al.[23] We have used the Wilson parameters given in Table 3 to correlate the excess Gibbs functions. According to this consistency test, the experimental data are considered thermodynamically consistent if the average deviation for the vapor phase composition is less than 0.01. We have obtained $\Delta y = 0.0099$ also for the mixtures containing 2-methyl-1-propanol or 2-methyl-2-propanol; consequently, the VLE data can be considered thermodynamically consistent.

The vapor pressure−liquid composition surface calculated with the Wilson equation for the two ternary systems is represented in Figures 1 and 2, respectively. These figures and our previous studies[8] show that p varies with liquid composition

Table 2. Isothermal VLE Data for the Binary and Ternary Mixtures: Experimental Vapor Pressure, p, Liquid-Phase, x_1, x_2, and Vapor-Phase, y_1, y_2, Mole Fractions, Correlated Activity Coefficients γ_i, and Excess Gibbs Functions, G^E

p (Pa)	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3	G^E (J·mol^{-1})
				2-Methyl-1-propanol (1) + n-Hexane (2)				
20510	0.0602	0.9398	0.0393	0.9607	8.010	1.028		375
20325	0.1250	0.8750	0.0449	0.9551	4.575	1.087		651
20255	0.1723	0.8277	0.0468	0.9532	3.482	1.139		801
19940	0.2734	0.7266	0.0499	0.9501	2.331	1.276		1012
19495	0.3753	0.6247	0.0533	0.9467	1.780	1.451		1113
19200	0.4310	0.5690	0.0556	0.9444	1.590	1.566		1128
18700	0.5111	0.4889	0.0597	0.9403	1.393	1.761		1106
17535	0.6132	0.3868	0.0643	0.9357	1.224	2.077		1009
15500	0.7234	0.2766	0.0856	0.9144	1.108	2.538		823
12485	0.8169	0.1831	0.1165	0.8835	1.046	3.077		602
7895	0.9122	0.0878	0.1782	0.8218	1.011	3.841		317
3885	0.9710	0.0290	0.3611	0.6389	1.001	4.473		111
			2-Methyl-1-propanol (1) + n-Hexane (2) + 1-Chlorobutane (3)					
8615	0.907	0.056	0.169	0.650	1.010	3.910	3.202	318
13170	0.623	0.084	0.090	0.352	1.174	2.533	1.936	920
13195	0.537	0.066	0.090	0.255	1.286	2.312	1.694	990
13530	0.428	0.065	0.084	0.202	1.503	2.049	1.460	1024
13380	0.350	0.046	0.080	0.144	1.746	1.917	1.324	978
13475	0.250	0.037	0.080	0.108	2.258	1.755	1.185	857
13490	0.163	0.026	0.055	0.057	3.099	1.643	1.092	666
15730	0.525	0.175	0.066	0.501	1.301	2.111	1.716	1069
15595	0.432	0.164	0.070	0.423	1.487	1.921	1.500	1096
15100	0.367	0.127	0.069	0.339	1.677	1.843	1.367	1055
14900	0.287	0.107	0.080	0.287	2.023	1.730	1.241	972
14475	0.212	0.077	0.063	0.182	2.552	1.653	1.145	827
17175	0.478	0.290	0.062	0.655	1.393	1.866	1.683	1140
18360	0.486	0.448	0.067	0.847	1.418	1.738	1.900	1139
18245	0.470	0.402	0.067	0.791	1.432	1.743	1.782	1156
17995	0.414	0.363	0.050	0.692	1.551	1.675	1.592	1172
17765	0.409	0.332	0.052	0.654	1.558	1.694	1.554	1166
17410	0.306	0.292	0.053	0.537	1.927	1.568	1.329	1107
16840	0.307	0.246	0.056	0.505	1.919	1.613	1.310	1087
16160	0.200	0.186	0.050	0.367	2.663	1.525	1.148	890
15720	0.202	0.155	0.050	0.328	2.643	1.557	1.144	872
14760	0.120	0.084	0.043	0.189	3.820	1.530	1.058	598
13915	0.101	0.025	0.052	0.062	4.247	1.570	1.041	478
18832	0.380	0.484	0.070	0.788	1.686	1.529	1.644	1168
18500	0.356	0.401	0.055	0.695	1.739	1.550	1.497	1167
19460	0.264	0.614	0.057	0.808	2.287	1.301	1.535	1072
19290	0.240	0.557	0.060	0.738	2.420	1.299	1.414	1061
19150	0.197	0.505	0.050	0.703	2.786	1.280	1.291	998
18620	0.173	0.419	0.053	0.591	3.030	1.308	1.201	939
18075	0.142	0.363	0.032	0.543	3.480	1.315	1.138	845
17200	0.119	0.268	0.040	0.446	3.892	1.365	1.085	732
16420	0.103	0.200	0.040	0.361	4.247	1.406	1.058	636
20070	0.152	0.815	0.046	0.918	3.807	1.121	1.598	772
20100	0.087	0.757	0.040	0.812	5.560	1.078	1.377	634
19950	0.128	0.682	0.050	0.767	4.077	1.134	1.350	800
19580	0.087	0.598	0.040	0.691	5.180	1.136	1.214	695
19180	0.090	0.516	0.024	0.651	4.928	1.178	1.161	711
18515	0.106	0.410	0.030	0.573	4.305	1.252	1.122	750
17800	0.103	0.326	0.030	0.497	4.319	1.307	1.088	709
17670	0.138	0.318	0.041	0.499	3.531	1.344	1.118	815
16415	0.104	0.200	0.030	0.367	4.221	1.407	1.059	639
15260	0.108	0.118	0.040	0.247	4.094	1.485	1.051	589
				2-Methyl-2-propanol (1) + n-Hexane (2)				
21585	0.1158	0.8842	0.1205	0.8795	3.969	1.049		501
21425	0.2126	0.7874	0.1515	0.8485	2.624	1.136		758
21250	0.2961	0.7039	0.1660	0.8340	2.043	1.237		895
20785	0.3826	0.6174	0.1802	0.8198	1.680	1.367		971
20050	0.4917	0.5083	0.2001	0.7999	1.397	1.577		981
19290	0.5763	0.4237	0.2195	0.7805	1.254	1.784		931
18590	0.6384	0.3616	0.2405	0.7595	1.177	1.968		865
17275	0.7159	0.2841	0.2620	0.7380	1.105	2.247		747
16125	0.7762	0.2238	0.3003	0.6997	1.064	2.511		630
14675	0.8243	0.1757	0.3403	0.6597	1.039	2.761		520
13420	0.8613	0.1387	0.3805	0.6195	1.024	2.981		426
10705	0.9204	0.0796	0.5002	0.4998	1.008	3.395		259
8050	0.9650	0.0350	0.6715	0.3285	1.002	3.770		119

Table 2. Continued

p /(Pa)	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3	G^E /(J·mol^{-1})
			2-Methyl-2-propanol (1) + n-Hexane (2) + 1-Chlorobutane (3)					
14595	0.714	0.091	0.301	0.269	1.084	2.555	2.064	704
15015	0.631	0.077	0.296	0.201	1.149	2.346	1.811	809
15115	0.549	0.063	0.288	0.158	1.241	2.173	1.610	873
15845	0.379	0.083	0.242	0.181	1.567	1.816	1.313	909
15855	0.284	0.071	0.210	0.141	1.905	1.698	1.188	823
15405	0.267	0.051	0.214	0.103	1.989	1.705	1.167	783
17175	0.523	0.180	0.231	0.368	1.274	1.929	1.611	958
17000	0.447	0.155	0.234	0.313	1.403	1.824	1.447	971
16875	0.365	0.135	0.224	0.265	1.603	1.721	1.307	941
16175	0.305	0.098	0.219	0.209	1.813	1.688	1.218	868
15780	0.270	0.055	0.214	0.120	1.973	1.703	1.171	791
19300	0.479	0.367	0.196	0.604	1.369	1.648	1.663	1021
18065	0.525	0.255	0.215	0.480	1.277	1.838	1.669	983
19505	0.503	0.405	0.186	0.678	1.341	1.659	1.767	1004
19675	0.406	0.390	0.189	0.603	1.522	1.518	1.523	1039
18920	0.296	0.304	0.160	0.471	1.855	1.449	1.277	975
18260	0.255	0.244	0.170	0.405	2.043	1.459	1.199	905
17550	0.207	0.192	0.159	0.328	2.337	1.464	1.132	801
16800	0.147	0.138	0.147	0.246	2.874	1.470	1.070	636
16195	0.090	0.095	0.114	0.182	3.678	1.479	1.029	440
14895	0.024	0.045	0.050	0.091	5.350	1.509	1.003	152
20675	0.318	0.561	0.150	0.726	1.855	1.307	1.518	985
19975	0.314	0.432	0.154	0.601	1.814	1.372	1.387	1008
20965	0.262	0.616	0.138	0.744	2.143	1.226	1.471	923
20805	0.244	0.559	0.138	0.681	2.208	1.231	1.381	925
20470	0.210	0.495	0.128	0.601	2.398	1.232	1.278	891
19965	0.174	0.426	0.125	0.549	2.665	1.243	1.191	826
19315	0.139	0.354	0.120	0.487	3.011	1.267	1.123	734
18500	0.111	0.276	0.109	0.411	3.366	1.311	1.075	629
17660	0.081	0.209	0.100	0.334	3.870	1.354	1.041	500
21430	0.096	0.866	0.109	0.847	4.339	1.039	1.508	470
21350	0.119	0.775	0.102	0.806	3.705	1.066	1.421	601
21070	0.110	0.699	0.105	0.733	3.745	1.079	1.326	626
20815	0.089	0.614	0.102	0.668	4.037	1.097	1.231	601
20155	0.071	0.522	0.086	0.603	4.331	1.129	1.155	561
19470	0.052	0.431	0.070	0.536	4.735	1.173	1.098	491
18620	0.040	0.340	0.061	0.461	5.007	1.230	1.059	421
17660	0.029	0.258	0.053	0.394	5.304	1.291	1.033	340
16320	0.015	0.162	0.032	0.286	5.763	1.377	1.012	218

Table 3. Correlation Parameters for the Wilson Equation and Average Deviation in Pressure, Δp

$\lambda_{12} - \lambda_{11}$/(J·mol^{-1}) $\lambda_{21} - \lambda_{22}$/(J·mol^{-1})	$\lambda_{13} - \lambda_{11}$/(J·mol^{-1}) $\lambda_{31} - \lambda_{33}$/(J·mol^{-1})	$\lambda_{23} - \lambda_{22}$/(J·mol^{-1}) $\lambda_{32} - \lambda_{33}$/(J·mol^{-1})	Δp/Pa
	2-Methyl-1-propanol (1) + n-Hexane (2) + 1-Chlorobutane (3)		
7382.46	5023.83	−590.32	106
749.73	910.05	1928.63	
	2-Methyl-2-propanol (1) + n-Hexane (2) + 1-Chlorobutane (3)		
5305.35	3974.44	−138.42	87
620.25	788.22	1360.45	

in a very similar way for the four ternary systems containing a butanol isomer + n-hexane + 1-chlorobutane: vapor pressure continuously diminishes when the mole fraction of butanol isomer increases in the mixture.

The G^E−liquid composition surfaces obtained with the Wilson equation for both ternary systems have been plotted in Figures 3 and 4, respectively. In these figures, we can observe that the G^E dependence with liquid composition is also very similar for the ternary systems containing a butanol isomer + n-hexane + 1-chlorobutane:[8] G^E values are positive and high in the full composition range, following the sequence 2-methyl-2-propanol < 2-butanol ≈ 1-butanol < 2-methyl-1-propanol. In previous papers, we have reported thermodynamic and transport properties such as excess molar volumes,[6] refractive index,[7] and viscosity deviations[6] for all the ternary systems. These studies have revealed that that the rupture of hydrogen bonds of butanol
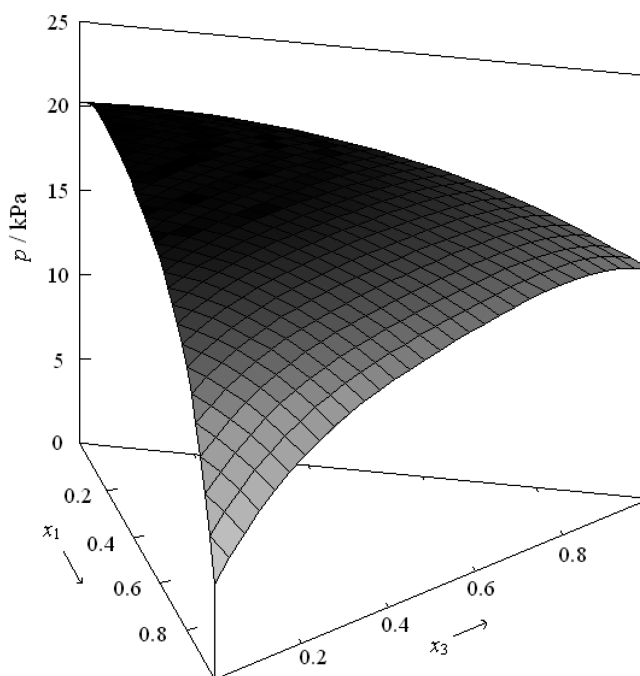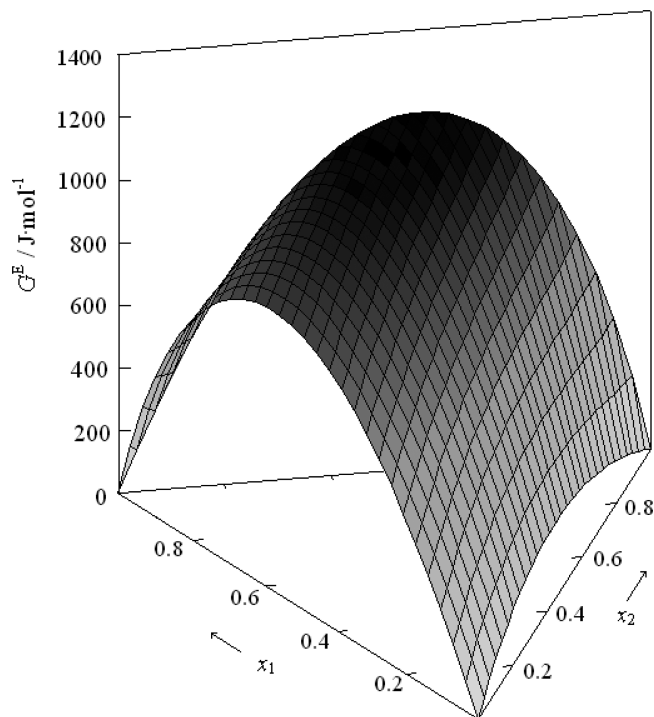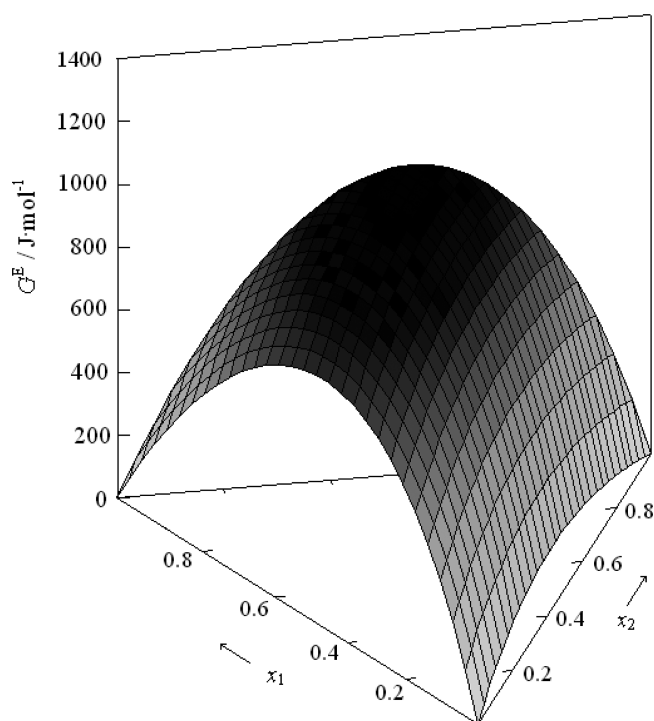

Figure 2. Vapor pressure−liquid composition surface calculated with the Wilson equation for the ternary system 2-methyl-2-propanol (1) + n-hexane (2) + 1-chlorobutane (3) at 298.15 K.

Figure 3. Excess Gibbs function−liquid composition surface obtained with the Wilson equation for the ternary system 2-methyl-1-propanol (1) + *n*-hexane (2) + 1-chlorobutane (3) at 298.15 K.

Figure 4. Excess Gibbs function−liquid composition surface obtained with the Wilson equation for the ternary system 2-methyl-2-propanol l (1) + *n*-hexane (2) + 1-chlorobutane (3) at 298.15 K.

isomers and the breaking of dipole−dipole interactions of 1-chlorobutane during the mixing process predominate over the formation of new interactions between molecules of butanol and chlorobutane. The same sequence for G^E values has been obtained in the VLE study of the binary systems butanol isomer + *n*-hexane at 298.15 K and shows that *n*-hexane is very efficient for breaking the hydrogen bonds of the pure butanols,

while butanol−chlorobutane interactions partially compensate the rupture of the self-interactions.

Supporting Information Available:

Composition dependence of density and speed of sound for the ternary systems 2-methyl-1-propanol + *n*-hexane + 1-chlorobutane and 2-methyl-2-propanol + *n*-hexane + 1-chlorobutane at 298.15 K is reported. These data have been used to analyze the composition of both liquid- and vapor-condensed phases. This material is available free of charge via the Internet at http://pubs.acs.org.

Literature Cited

(1) Dominguez, M.; Artigas, H.; Santafe, J.; Mainar, A.; Urieta, J. S. Densities and excess molar volumes of the ternary mixture (1-butanol plus n-hexane plus 1-chlorobutane) at 298.15 and 313.15 K. Application of the ERAS model. *Fluid Phase Equilib.* **1998**, *145*, 115–128.

(2) Dominguez, M.; Santafe, J.; Lopez, M. C.; Royo, F. M.; Urieta, J. S. Viscosities of the ternary mixture (1-butanol plus n-hexane plus 1-chlorobutane) at 298.15 and 313.15 K. *Fluid Phase Equilib.* **1998**, *152*, 133–148.

(3) Dominguez, M.; Lafuente, C.; Lopez, M. C.; Royo, F. M.; Urieta, J. S. Speed of sound and isentropic compressibility of (1-butanol plus n-hexane plus 1-chlorobutane) and the constituent binary mixtures at the temperatures 298.15 and 313.15 K. *J. Chem. Thermodyn.* **2000**, *32*, 155–173.

(4) Dominguez, M.; Martin, S.; Santafe, J.; Artigas, H.; Royo, F. M. Densities and speeds of sound in the ternary mixture (2-butanol plus n-hexane plus 1-chlorobutane) at 298.15 and 313.15 K. *Thermochim. Acta* **2002**, *381*, 181–193.

(5) Dominguez, M.; Langa, E.; Mainar, A. M.; Santafe, J.; Urieta, J. S. Measurements, correlations, and predictions of viscosities for the ternary mixture (2-butanol plus hexane plus 1-chlorobutane) at 298.15 and 313.15 K. *J. Chem. Eng. Data* **2003**, *48*, 302–307.

(6) Carrasco, A.; Perez-Navarro, M.; Gascon, I.; Lopez, M. C.; Lafuente, C. Densities and viscosities of the ternary mixtures 2-methyl-1-propanol (or 2-methyl-2-propanol) plus n-hexane plus 1-chlorobutane at 298.15 K. *J. Chem. Eng. Data* **2008**, *53*, 1223–1227.

(7) Perez-Navarro, M.; Pera, G.; Haro, M.; Gascon, I.; Lafuente, C. Refractive Indices of the Ternary Mixtures Butanol + n-Hexane + 1-Chlorobutane. *J. Solution Chem.* **2008**, *37*, 1499–1510.

(8) Martinez, S.; Bandres, I.; Ballesteros, L. M.; Lafuente, C.; Gascon, I. (Vapour + liquid) equilibrium and excess Gibbs functions of ternary mixtures containing 1-butanol or 2-butanol, n-hexane, and 1-chlorobutane at T = 298.15 K. *J. Chem. Thermodyn.* **2009**, *41*, 1030–1034.

(9) Van Ness, H. C.; Byer, S. M.; Gibbs, R. E. Vapor-liquid equilibria. I. Appraisal of data reduction methods. *AIChE J.* **1973**, *19*, 238–244.

(10) Wilson, G. M. A new expression for the excess Gibbs free energy of mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127–130.

(11) Berro, C.; Rogalski, M.; Peneloux, A. Excess Gibbs energies and excess volumes of 1-butanol + n-hexane and 2-methyl-1-propanol + n-hexane binary systems. *J. Chem. Eng. Data* **1982**, *27*, 352–355.

(12) Rodriguez, V.; Pardo, J.; Lopez, M. C.; Royo, F. M.; Urieta, J. S. Vapor pressures of binary mixtures of hexane + 1-butanol, + 2-butanol, + 2-methyl-1-propanol, or + 2-methyl-2-propanol at 298.K. *J. Chem. Eng. Data* **1993**, *38*, 350–352.

(13) Janaszewski, B.; Oracz, P.; Goral, M.; Warycha, S. Vapour-liquid equilibria. I. An apparatus for isothermal total vapour pressure measurements: binary mixtures of ethanol or t-butanol with n-hexane, n-heptane and n-octane. *Fluid Phase Equilib.* **1982**, *9*, 295–310.

(14) Garriga, R.; Martinez, S.; Perez, P.; Gracia, M. Thermodynamic excess properties for binary mixtures of 1-chlorobutane with 2-butanol or 2-methyl-1-propanol. *Fluid Phase Equilib.* **2001**, *181*, 203–214.

(15) Garriga, R.; Martinez, S.; Perez, P.; Gracia, M. Isothermal (vapour + liquid) equilibrium at several temperatures of (1-chlorobutane + 1-butanol, or 2-methyl-2-propanol). *J. Chem. Thermodyn.* **2001**, *33*, 523–534.

(16) Gutsche, B.; Knapp, H. Isothermal measurements of vapour liquid equilibria for 3 normal-alkane chloroalkane mixtures. *Fluid Phase Equilib.* **1982**, *8*, 285–300.

(17) Perez-Gregorio, V.; Montaño, D.; Giner, B.; Lafuente, C.; Royo, F. M. Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures. *J. Chem. Thermodyn.* **2009**, *41*, 553–559.

(18) Nain, A. K.; Sharma, R.; Ali, A.; Gopal, S. Densities and volumetric properties of ethyl acrylate + 1-butanol, or 2-butanol, or 2-methyl-1-propanol, or 2-methyl-2-propanol binary mixtures at temperatures from 288.15 to 318.15 K. *J. Mol. Liq.* **2009**, *144*, 138–144.

(19) Moravkova, L.; Linek, J. Excess molar volumes of (octane + 1-chlorobutane) at temperatures between 298.15 and 328.15K and at pressures up to 40 MPa. *J. Chem. Thermodyn.* **2003**, *35*, 113–121.

(20) Silverman, N.; Tassios, D. P. Prediction of multicomponent VLE with the Wilson equation. Effect of the minimization function and of the quality of binary data. *Ind. Eng. Chem. Process. Des. Dev.* **1984**, *23*, 586–589.

(21) *TRC Thermodynamic Tables-Non-Hydrocarbons, Selected Values of Properties of Chemical Compounds*; Thermodynamic Research Center, Texas A&M University: College Station, TX.

(22) Amdur, I.; Mason, E. A. Properties of gases at very high temperatures. *Phys. Fluids* **1958**, *1*, 370–383.

(23) Fredenslund, A.; Gmehling, J.; Rasmussen, P. *Vapor-Liquid Equilibria Using UNIFAC*; Elsevier: Amsterdam, 1977.