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(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

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ABSTRACT

Isothermal (vapour + liquid) equilibrium data for the ternary mixtures 1-butanol + n-hexane + 1-chlorobutane and 2-butanol + n-hexane + 1-chlorobutane have been studied with a recirculating still at $T = 298.15$ K. The experimental data were satisfactorily checked for thermodynamic consistency using the method of van Ness. Activity coefficients and excess Gibbs function have been correlated with the Wilson equation. The G^E values obtained for the two ternary systems are very similar.

1. Introduction

Isothermal (vapour + liquid) equilibrium data of multicomponent mixtures are of great interest for the developing of different methods to predict and correlate phase equilibrium and also in order to understand further the molecular interactions between components of liquid mixtures. In the last years our laboratory has been involved in the study of thermodynamic and transport properties of ternary mixtures [1–12] containing different organic compounds (isomers of butanol, cyclic ethers, alkanes, and chloroalkanes). Following these systematic studies we present here (vapour + liquid) equilibrium data obtained at the temperature of 298.15 K for the ternary mixtures 1-butanol (or 2-butanol) + n-hexane + 1-chlorobutane. Thermodynamic consistency of the experimental data has been checked by the method of van Ness. We also have correlated activity coefficients of the components and excess Gibbs function of the mixtures using the Wilson equation [13].

To 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: 1-butanol + n-hexane [14–19], 2-butanol + n-hexane [19–22], 1-butanol or 2-butanol + 1-chlorobutane [23,24], and n-hexane + 1-chlorobutane [25,26].

Previously the isobaric VLE data for the ternary systems at 101.3 kPa have been reported [3,8], a good agreement between the studies performed in both conditions (isothermal and isobaric data) has been observed.

2. Experimental section

To obtain the isothermal (vapour + liquid) equilibrium of the systems studied, the compounds 1-butanol (purity better than 99.8 mol%), 2-butanol, n-hexane, and 1-chlorobutane (better than 99 mol%) were obtained from Aldrich. The alcohols, 1-butanol and 2-butanol, were stored under activated molecular sieve. The purity of the chemicals was checked by comparing experimental densities and pressures at the temperature of 298.15 K with those reported in the literature [24,27]. No further purification was considered necessary. Densities were measured with an Anton Paar DMA-5000 vibrating tube densimeter. The measured vapour pressures and densities of the pure compounds are collected in table 1.

The (vapour + 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 temperature was 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 in order to obtain the desired boiling

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TABLE 1
Properties of the pure compounds at $T = 298.15$ K.

Compound	p^{exp}/kPa	p^{lit}/kPa	$\rho^{exp}/(kg \cdot m^{-3})$	$\rho^{lit}/(kg \cdot m^{-3})$	$B \times 10^6/(m^3 \cdot mol^{-1})$
1-Butanol	0.910	0.910 [27]	805.802	805.75 [27]	−6496 [29]
2-Butanol	2.340	2.324 [24]	802.451	802.41 [27]	−4474 [29]
n-Hexane	20.22	20.17 [27]	654.960	654.84 [27]	−1919 [29]
1-Chlorobutane	13.515	13.499 [27]	880.805	880.95 [27]	−1722 [29]

TABLE 2
Isothermal VLE data for the ternary mixtures: experimental vapour pressure, p, liquid-phase, x_1, x_2 and vapour phase, y_1, y_2 mole fractions, correlated activity coefficients γ_i, and excess Gibbs function, G^E.

p/kPa	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3	$G^E/(J \cdot mol^{-1})$
			{1-Butanol (1) + n-hexane (2) + 1-chlorobutane (3)}					
6.405	0.886	0.033	0.121	0.404	1.012	4.127	2.717	343
10.025	0.827	0.094	0.087	0.649	1.031	3.527	2.513	536
13.210	0.759	0.170	0.067	0.758	1.069	2.975	2.320	733
15.065	0.701	0.233	0.036	0.821	1.114	2.612	2.183	871
16.630	0.627	0.314	0.039	0.867	1.193	2.246	2.040	1009
17.515	0.558	0.389	0.035	0.890	1.294	1.976	1.929	1100
18.015	0.512	0.442	0.036	0.909	1.382	1.823	1.869	1140
18.655	0.447	0.517	0.031	0.925	1.542	1.640	1.796	1166
19.090	0.370	0.605	0.035	0.941	1.810	1.463	1.722	1149
19.345	0.307	0.678	0.030	0.955	2.132	1.343	1.674	1092
11.105	0.711	0.059	0.076	0.324	1.082	3.146	2.094	727
13.180	0.673	0.119	0.045	0.499	1.112	2.804	2.010	842
15.455	0.608	0.204	0.028	0.633	1.181	2.389	1.886	988
16.385	0.566	0.265	0.034	0.709	1.241	2.166	1.826	1063
17.395	0.509	0.340	0.033	0.764	1.341	1.927	1.752	1133
18.110	0.449	0.421	0.036	0.812	1.485	1.719	1.690	1174
18.540	0.401	0.485	0.037	0.839	1.632	1.583	1.649	1181
18.955	0.349	0.555	0.033	0.867	1.843	1.457	1.615	1161
19.275	0.289	0.605	0.030	0.868	2.156	1.347	1.546	1111
19.505	0.239	0.705	0.031	0.914	2.606	1.246	1.564	1014
12.690	0.523	0.056	0.065	0.206	1.266	2.510	1.624	939
14.890	0.475	0.135	0.054	0.400	1.350	2.189	1.550	1038
16.300	0.433	0.222	0.037	0.521	1.447	1.935	1.509	1112
17.565	0.370	0.332	0.019	0.628	1.647	1.670	1.458	1158
18.265	0.324	0.419	0.031	0.697	1.851	1.514	1.439	1157
18.905	0.277	0.510	0.030	0.756	2.142	1.381	1.431	1121
19.380	0.233	0.601	0.030	0.801	2.530	1.278	1.438	1051
19.765	0.180	0.702	0.029	0.858	3.228	1.180	1.453	921
20.045	0.120	0.801	0.026	0.902	4.667	1.096	1.467	715
14.005	0.306	0.087	0.045	0.215	1.827	1.924	1.264	950
14.750	0.293	0.112	0.047	0.273	1.886	1.854	1.251	963
16.340	0.269	0.206	0.041	0.420	2.033	1.663	1.243	1016
17.150	0.242	0.287	0.025	0.499	2.226	1.525	1.239	1030
17.915	0.224	0.361	0.028	0.576	2.406	1.425	1.249	1033
18.410	0.199	0.427	0.028	0.615	2.680	1.341	1.253	1006
18.950	0.173	0.504	0.030	0.675	3.060	1.260	1.269	959
19.250	0.146	0.584	0.035	0.724	3.601	1.190	1.292	886
19.720	0.113	0.675	0.019	0.785	4.556	1.122	1.326	765
20.000	0.085	0.758	0.019	0.818	5.873	1.075	1.371	630
14.495	0.096	0.092	0.070	0.189	4.150	1.590	1.044	534
15.135	0.094	0.104	0.050	0.201	4.212	1.570	1.044	539
16.390	0.092	0.200	0.042	0.343	4.360	1.439	1.058	616
17.185	0.086	0.276	0.048	0.444	4.653	1.351	1.073	645
17.605	0.080	0.327	0.042	0.472	4.957	1.298	1.085	647
18.130	0.073	0.383	0.033	0.520	5.319	1.246	1.102	644
18.650	0.066	0.452	0.030	0.578	5.852	1.192	1.128	629
19.485	0.031	0.608	0.021	0.688	9.377	1.088	1.200	460
19.970	0.011	0.736	0.010	0.778	14.356	1.036	1.298	298
			{2-Butanol (1) + n-hexane (2) + 1-chlorobutane (3)}					
7.075	0.899	0.027	0.305	0.315	1.010	4.306	2.632	298
12.505	0.799	0.123	0.171	0.632	1.049	3.273	2.252	612
14.400	0.752	0.181	0.145	0.710	1.082	2.881	2.115	746
17.415	0.610	0.332	0.105	0.802	1.231	2.113	1.845	1018
19.165	0.407	0.558	0.082	0.877	1.693	1.487	1.674	1125
20.155	0.202	0.777	0.068	0.920	3.040	1.148	1.651	849
20.205	0.200	0.721	0.063	0.847	2.929	1.165	1.541	891
20.325	0.146	0.799	0.057	0.886	3.797	1.095	1.585	726
11.945	0.702	0.054	0.163	0.266	1.084	3.008	2.029	715
13.905	0.663	0.117	0.129	0.448	1.120	2.686	1.920	829
15.945	0.596	0.207	0.094	0.583	1.197	2.285	1.780	972

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