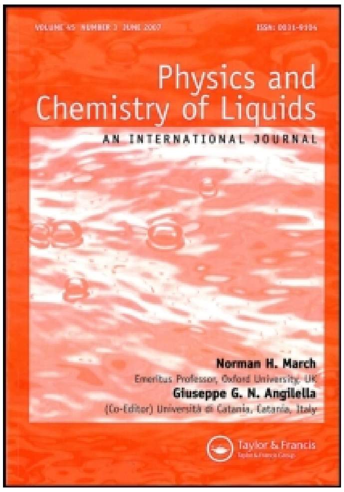

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Vapour-Liquid equilibrium and volumetric measurements for binary mixtures of 1,3-Dioxolane with Isomeric chlorobutanes

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VAPOUR–LIQUID EQUILIBRIUM AND VOLUMETRIC MEASUREMENTS FOR BINARY MIXTURES OF 1,3-DIOXOLANE WITH ISOMERIC CHLOROBUTANES

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Isobaric vapour–liquid equilibrium measurements for 1,3-dioxolane with isomeric chlorobutane at 40.0 and 101.3 kPa are reported. Activity coefficients were calculated from experimental data. The VLE measurements are thermodynamically consistent. Margules, Van Laar, Wilson, NRTL and UNIQUAC equations have been used to correlate the activity coefficients and we have obtained satisfactory results. We also present density measurements of these systems at 298.15 K.

Keywords: 1,3-Dioxolane; Chlorobutane; Isobaric vapour–liquid equilibrium

INTRODUCTION

In recent studies we have reported thermodynamic and transport properties for several mixtures containing cyclic ethers [1] and haloalkanes [2,3]. We have obtained very useful information from these kinds of systems, following on our study we present here isobaric vapour–liquid equilibrium (VLE) and densities for binary mixtures of 1,3-dioxolane with isomeric chlorobutane. Densities have been determined at 298.15 K and results have been fitted by means of a polynomial type equation. Isobaric VLE has been measured at 40.0 kPa (except for 2-chloro-2-methyl-propane due to its low boiling temperature) and 101.3 kPa. VLE experimental results have been checked for thermodynamic consistency with van Ness method [4].

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TABLE I Densities (ρ) at 298.15 K and normal boiling points (T_b) of pure liquids

Compound	ρ (g cm^{-3})		T_b (K)	
	Exptl	*Lit*	*Exptl*	*Lit*
1,3-Dioxolane	1.05898	1.05866[a]	348.55	348.80[b]
1-Chlorobutane	0.88067	0.88095[a]	351.58	351.58[a]
2-Chlorobutane	0.86726	0.86710[a]	341.40	341.40[a]
1-Chloro-2-methylpropane	0.87094	0.87170[a]	342.10	342.00[a]
2-Chloro-2-methylpropane	0.83693	0.83610[a]	323.83	323.90[a]

[a]Ref. [10]; [b]Ref. [11].

Activity coefficients obtained from experimental data have been correlated with Margules [5], Van Laar [6], Wilson [7], NRTL [8] and UNIQUAC [9] equations.

We have not found any isobaric VLE study on literature involving these mixtures.

EXPERIMENTAL

All liquids used on the determination of the experimental measurements were provided from Aldrich (1-chlorobutane, 2-chloro-2-methylpropane and 1,3-dioxolane with a purity of 99% while 2-chlorobutane with purity better than 99%), excepting 1-chloro-2-methylpropane from Fluka (purity better than 98%). In Table I the comparison between experimental data of densities at 298.15 K and normal boiling point with literature values [10,11] is given.

Densities have been measured with an Anton Paar DMA 58 vibrating tube densimeter automatically thermostated at 298.15 ± 0.01 K. Calibration was carried out with deionised doubly distilled water and dry air. The precision of density measurements is estimated to be $\pm 5 \times 10^{-6}$ g cm^{-3}.

Experimental data of VLE was performed using an all-glass, dynamic recirculating still Fischer-Labodest model equipped with a Cottrell pump, a pressure transducer Druk PDCR 110/W and a thermometer from Automatic System Laboratories (model F25). The accuracy of the thermometer is estimated to be ± 0.01 K while the accuracy of pressure transducer is ± 0.1 kPa. Experimental procedure has been previously described [12]. Composition of both phases has been determined by density measurements. The error in the determination of liquid and vapour phases is estimated to be ± 0.0001.

RESULTS AND DISCUSSION

Experimental data for densities of the mixtures are shown in Table II and they are graphically represented in Fig. 1. Values have been correlated by means of a polynomial equation:

$$\rho = x_1\rho_1^0 + (1 - x_1)\rho_2^0 + x_1(1 - x_1)\sum_{i=1}^{n} A_i(2x_1 - 1)^2 \qquad (1)$$

TABLE II Densities (ρ) at 298.15 K of the binary mixtures studied

x_1	ρ (g cm^{-3})	x_1	ρ (g cm^{-3})	x_1	ρ (g cm^{-3})
1,3-Dioxolane (1) + 1-chlorobutane (2)					
0.0464	0.88607	0.4574	0.94293	0.8265	1.01505
0.0703	0.88890	0.5410	0.95718	0.9131	1.03598
0.2214	0.90792	0.6565	0.97877	0.9577	1.04744
0.3225	0.92204	0.7291	0.99357		
1,3-Dioxolane (1) + 2-chlorobutane (2)					
0.1094	0.88169	0.5546	0.95400	0.8284	1.01355
0.2962	0.90906	0.6010	0.96313	0.9033	1.03255
0.4537	0.93532	0.6945	0.98264	0.9497	1.04494
1,3-Dioxolane (1) + 1-chloro-2-methylpropane (2)					
0.0348	0.87525	0.3956	0.92715	0.7950	1.00627
0.0931	0.88270	0.4975	0.94481	0.9022	1.03264
0.1943	0.89639	0.5996	0.96414	0.9485	1.04474
0.2983	0.91166	0.6941	0.98361		
1,3-Dioxolane (1) + 2-chloro-2-methylpropane (2)					
0.0226	0.84061	0.4217	0.91179	0.8055	1.00210
0.1024	0.85355	0.5027	0.92887	0.9087	1.03118
0.1975	0.86957	0.6086	0.95272	0.9488	1.04319
0.3114	0.89016	0.7026	0.97531		

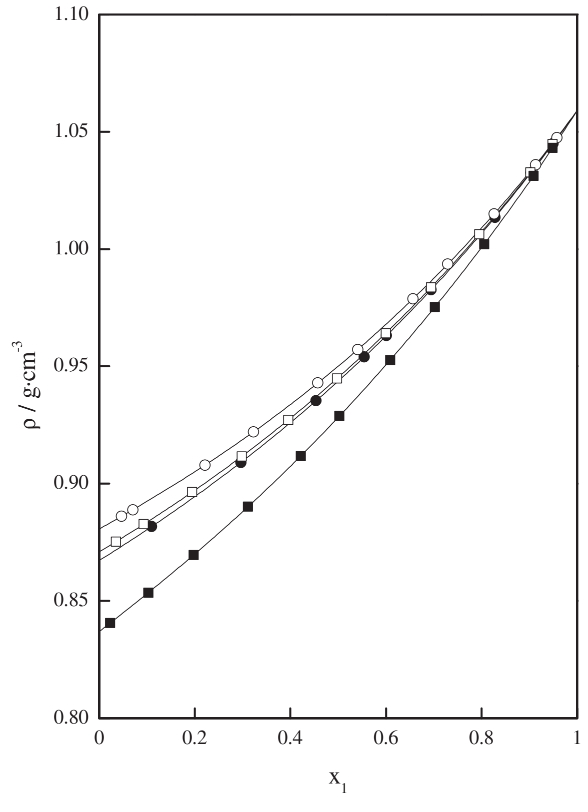

FIGURE 1 Densities for 1,3-dioxolane (1) with an isomeric chlorobutane (2) at $T = 298.15$ K as a function of mole fraction x_1. 1-Chlorobutane (□); 2-chlorobutane (■); 2-methyl-1-chloropropane (○); 2-methyl-2-chloropropane (●).

TABLE III Density correlation coefficients A_i

System	A_1	A_2	A_3	A_4
1,3-Dioxolane +				
1-chlorobutane	−0.07905	−0.01486	−0.00233	−0.00342
2-Chlorobutane	−0.07768	−0.01495	−0.00150	0.00060
1-Chloro-2-methylpropane	−0.07875	−0.01312	−0.00084	−0.00112
2-Chloro-2-methylpropane	−0.07887	−0.01202	−0.00023	−0.00441

where ρ_i^0 are the densities of pure compounds. Coefficients A_i are adjustable parameters and they have been gathered in Table III.

Vapour–liquid equilibrium experimental values, T, x_1, y_1 together with the calculated activity coefficients, γ_i, of studied systems are listed in Table IV and their corresponding graphics are represented in Figs. 2–5. Activity coefficients γ_i have been calculated by means of the equations below:

$$\gamma_i = \frac{y_i p}{x_i p_i^0} \exp\left[\frac{(B_{ii} - V_i^0)(P - P_i^0) + (1 - y_i)^2 P\delta_{ij}}{RT}\right] \tag{2}$$

$$\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj} \tag{3}$$

where x_i and y_i are liquid and vapour phase compositions, P is the total pressure, P_i^0 are vapour pressures of the pure compounds calculated from Antoine's equation [10,13,14]. Coefficients of these constants are given in Table V. B_{ii} are second virial coefficients and B_{ij} are cross second virial coefficients calculated using a mixing rule. V_I^0 is molar volume of saturated pure liquid which were calculated from Yen and Woods method [15]. The exponential term in Eq. (2) was important only at the extreme concentrations.

Thermodynamic consistency of the activity coefficients was tested using van Ness Method by means of a third-order Legendre polynomial for the excess Gibbs energies [16]. This method considers that experimental data are thermodynamically consistent if mean absolute deviation between calculated and measured vapour phase compositions, Δy, is lower than 0.01. All our mixtures are thermodynamically consistent and values of Δy are shown in Table VI.

Activity coefficients were correlated with Margules, Van Laar, Wilson, NRTL and UNIQUAC equations. Calculation of parameters for equations was based on minimising of the following objective function:

$$F = \sum_{k=1}^{N} \sum_{i=1}^{2} \left(\frac{\gamma_i^{\text{exptl}} - \gamma_i^{\text{cal}}}{\gamma_i^{\text{exptl}}}\right)^2 \tag{4}$$

which was formulated by Silvermann and Tassios [17] and where N is the number of experimental data points. Minimisation of F has been done with a non-linear regression procedure [18].

Correlation parameters, A_{ij} and A_{ji}, average deviations in temperature and vapour phase composition, ΔT and Δy, and activity coefficients at infinite dilution, γ_i^∞ and γ_j^∞ are gathered in Table VII. We can consider satisfactory that all the correlations and deviations are similar for every mixture with all the equations. Temperature

TABLE IV VLE experimental values of temperature (T), mole fraction of liquid phase and vapour phase, x_1 and y_1 and activity coefficients, γ_i, of the mixtures formed by 1,3-dioxolane (1) with isomeric chlorobutane (2) at 40.0 and 101.3 kPa

T (K)	x_1	y_1	γ_1	γ_2
1,3-Dioxolane (1) + 1-chlorobutane (2) at 40.0 kPa				
323.83	0.0419	0.0582	1.346	1.000
323.32	0.0814	0.1155	1.403	0.998
322.50	0.1584	0.2073	1.337	1.007
321.91	0.2411	0.2945	1.277	1.016
321.21	0.3470	0.3897	1.208	1.049
320.81	0.4573	0.4801	1.147	1.092
320.70	0.5101	0.5221	1.123	1.116
320.62	0.6073	0.5954	1.080	1.183
320.71	0.6672	0.6425	1.057	1.229
320.97	0.7200	0.6845	1.032	1.276
321.35	0.8210	0.7756	1.010	1.400
321.81	0.9002	0.8599	1.003	1.540
322.62	0.9609	0.9405	0.995	1.620
1,3-Dioxolane (1) + 1-chlorobutane (2) at 101.3 kPa				
350.67	0.0391	0.0573	1.368	1.008
350.10	0.0821	0.1152	1.334	1.008
349.08	0.1554	0.2046	1.294	1.016
348.07	0.2450	0.3024	1.254	1.028
347.21	0.3464	0.3989	1.203	1.051
346.77	0.4567	0.4886	1.134	1.091
346.50	0.5084	0.5322	1.119	1.112
346.45	0.6066	0.6077	1.073	1.167
346.42	0.6640	0.6546	1.057	1.204
346.58	0.7294	0.7087	1.036	1.255
346.80	0.8258	0.7951	1.019	1.362
347.36	0.8955	0.8666	1.006	1.452
348.06	0.9613	0.9459	1.000	1.557
1,3-Dioxolane (1) + 2-chlorobutane (2) at 40.0 kPa				
314.54	0.0583	0.0620	1.505	0.985
314.43	0.1251	0.1315	1.495	0.985
314.38	0.2497	0.2276	1.299	1.024
314.65	0.3420	0.3023	1.245	1.044
315.28	0.4893	0.4075	1.142	1.116
316.07	0.6022	0.4926	1.086	1.192
316.57	0.6578	0.5375	1.062	1.240
317.69	0.7556	0.6262	1.028	1.347
318.44	0.8052	0.6807	1.017	1.405
319.06	0.8409	0.7208	1.005	1.471
320.10	0.8924	0.7960	1.003	1.531
321.41	0.9433	0.8774	0.992	1.667
1,3-Dioxolane (1) + 2-chlorobutane (2) at 101.3 kPa				
340.70	0.0577	0.0634	1.430	1.010
340.58	0.1251	0.1315	1.373	1.013
340.52	0.2406	0.2352	1.280	1.029
340.52	0.3436	0.3203	1.220	1.058
341.01	0.4803	0.4275	1.146	1.109
341.84	0.6073	0.5219	1.075	1.195
342.35	0.6582	0.5687	1.062	1.220
343.35	0.7595	0.6587	1.031	1.331
344.00	0.8030	0.7076	1.024	1.366
344.50	0.8359	0.7457	1.020	1.405
345.61	0.8934	0.8177	1.008	1.500
346.92	0.9435	0.8973	1.003	1.534

(*continued*)

TABLE IV Continued

T (K)	x_1	y_1	γ_1	γ_2
1,3-Dioxolane (1) + 1-chloro-2-methylpropane (2) at 40.0 kPa				
315.31	0.0196	0.0197	1.377	1.000
315.24	0.0602	0.0707	1.614	0.992
315.23	0.0831	0.0905	1.497	0.995
315.20	0.1339	0.1400	1.439	0.997
315.12	0.1854	0.1922	1.432	0.999
315.12	0.2400	0.2340	1.346	1.015
315.16	0.2711	0.2592	1.318	1.022
315.34	0.2965	0.2795	1.290	1.023
315.51	0.3664	0.3304	1.225	1.049
315.72	0.4348	0.3879	1.201	1.067
316.07	0.5085	0.4329	1.130	1.122
316.38	0.5604	0.4754	1.111	1.147
316.69	0.6035	0.5092	1.091	1.176
317.22	0.6672	0.5595	1.061	1.233
318.25	0.7717	0.6586	1.035	1.341
318.88	0.8061	0.6944	1.018	1.381
320.41	0.8934	0.8031	0.998	1.530
322.48	0.9743	0.9439	0.990	1.679
1,3-Dioxolane (1) + 1-chloro-2-methylpropane (2) at 101.3 kPa				
341.63	0.0193	0.0211	1.378	1.012
341.49	0.0806	0.0922	1.448	1.006
341.35	0.1304	0.1425	1.390	1.009
341.04	0.1840	0.1842	1.287	1.033
341.15	0.2040	0.2126	1.335	1.018
341.12	0.2369	0.2429	1.315	1.022
341.03	0.2721	0.2417	1.143	1.076
341.13	0.2961	0.2928	1.268	1.035
341.28	0.3700	0.3397	1.171	1.075
341.74	0.5069	0.4586	1.136	1.110
342.03	0.5567	0.4971	1.110	1.137
342.84	0.6588	0.5846	1.073	1.190
343.32	0.7199	0.6330	1.046	1.262
343.87	0.7633	0.6656	0.957	1.499
345.22	0.8493	0.7752	1.018	1.357
345.88	0.8944	0.8287	1.011	1.447
346.99	0.9401	0.8949	1.002	1.514
347.78	0.9679	0.9452	1.001	1.440
1,3-Dioxolane (1) + 2-chloro-2-methylpropane (2) at 101.3 kPa				
324.87	0.0897	0.0539	1.396	1.005
325.95	0.1850	0.1100	1.325	1.021
327.50	0.2971	0.1756	1.241	1.045
328.71	0.3794	0.2267	1.198	1.070
331.75	0.5464	0.3331	1.091	1.151
334.26	0.6629	0.4304	1.061	1.227
336.41	0.7453	0.5083	1.031	1.317
338.79	0.8159	0.5924	1.009	1.411
340.56	0.8673	0.6700	1.010	1.507
341.94	0.8923	0.7266	1.015	1.480
344.43	0.9398	0.8193	0.999	1.635
346.30	0.9653	0.8952	0.998	1.563

deviations are between 0.05 and 0.24 K while deviations in composition are between 0.0025 and 0.0075.

We have chosen Wilson equation to obtain T, x, y diagrams, which are graphically represented for all the mixtures at 101.13 and 40.0 kPa in Figs. 2–5 together with experimental data.

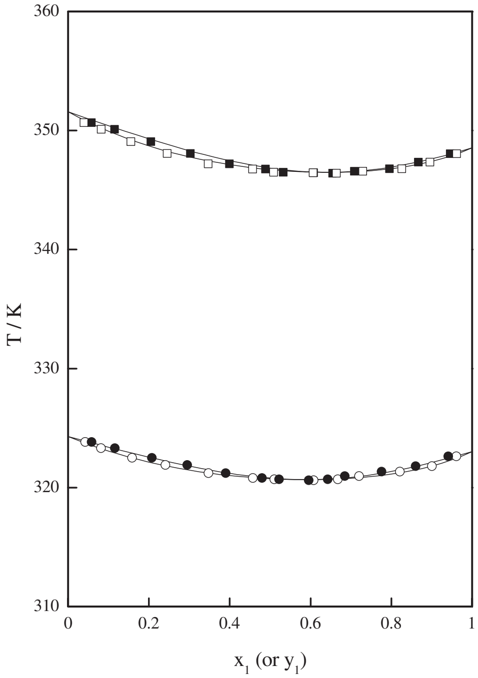

FIGURE 2 *T*, *x*, *y* diagram for 1,3-dioxolane (1) + 1-chlorobutane (2): (○, ●) exptl data at 40.0 kPa; (□, ■) exptl data at 101.3 kPa; (————) Wilson equation.

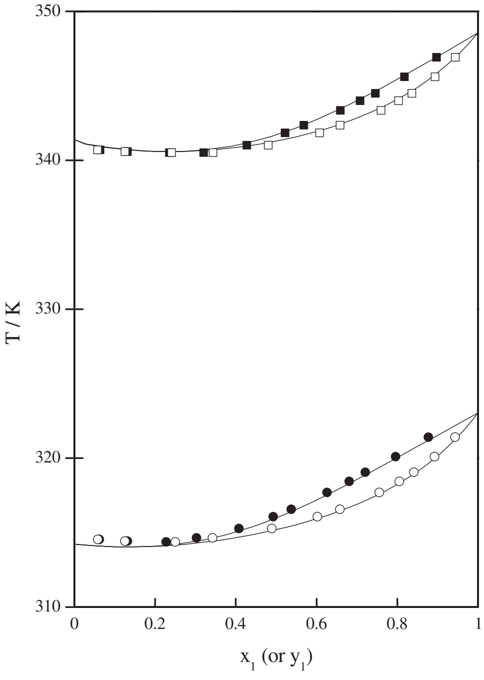

FIGURE 3 *T*, *x*, *y* diagram for 1,3-dioxolane (1) + 2-chlorobutane (2): (○, ●) exptl data at 40.0 kPa; (□, ■) exptl data at 101.3 kPa; (————) Wilson equation.

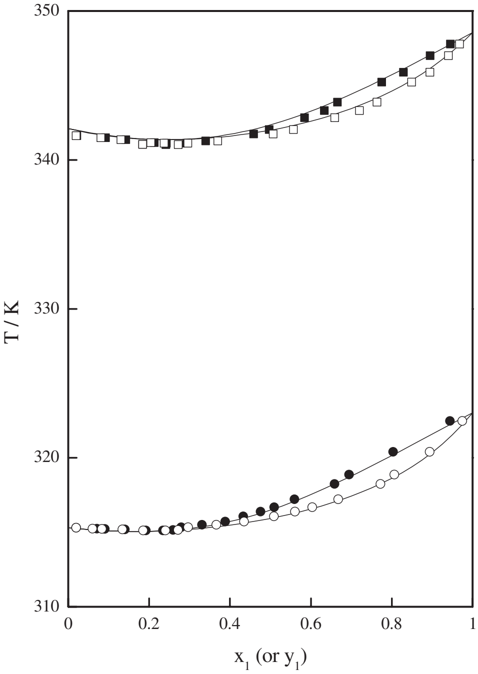

FIGURE 4 *T*, *x*, *y* diagram for 1,3-dioxolane (1) + 1-chloro-2-methylpropane (2): (○, ●) exptl data at 40.0 kPa; (□, ■) exptl data at 101.3 kPa; (————) Wilson equation.

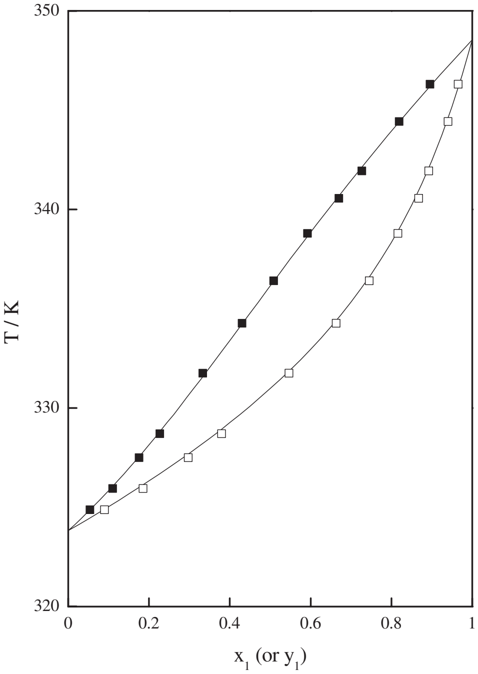

FIGURE 5 *T*, *x*, *y* diagram for 1,3-dioxolane (1) + 2-chloro-2-methylpropane (2): (□, ■) exptl data at 101.3 kPa; (————) Wilson equation.

TABLE V Coefficients of Antoine's equation for pure compounds (pressure in kPa and temperature in °C)

Compound	*A*	*B*	*C*
1,3-Dioxolane[a]	6.23182	1236.700	217.235
1-Chlorobutane[b]	6.05154	1216.820	222.330
2-Chlorobutane[b]	6.12220	1245.200	234.400
1-Chloro-2-methylpropane[c]	6.01854	1176.060	224.125
2-Chloro-2-methylpropane[c]	5.99201	114.899	229.000

[a]Ref. [13]; [b]Ref. [10]; [c]Ref. [14].

TABLE VI Values of average deviations ΔP and Δy obtained from the test of the thermodynamic consistence

System	P (kPa)	ΔP (kPa)	Δy
1,3-Dioxolane +			
1-Chlorobutane	40.0	0.09	0.0046
	101.3	0.36	0.0036
2-Chlorobutane	40.0	0.30	0.0027
	101.3	0.48	0.0028
1-Chloro-2-methylpropane	40.0	0.21	0.0027
	101.3	0.86	0.0052
2-Chloro-2-methylpropane	101.3	0.43	0.0041

TABLE VII Correlation parameters, A_{ij} and A_{ji}, average deviations, ΔT and Δy, and activity coefficients at infinite dilution, γ_i^∞ and γ_j^∞

Equation	A_{ij}	A_{ji}	ΔT (K)	Δy	γ_i^∞	γ_j^∞
1,3-Dioxolane (1) + 1-chlorobutane (2) at 40.0 kPa						
Margules	0.3549	0.5418	0.05	0.0048	1.43	1.72
Van Laar	0.3720	0.5498	0.06	0.0046	1.45	1.73
Wilson	777.8019	718.1191	0.06	0.0046	1.40	1.66
NRTL	2392.7756	−842.8840	0.06	0.0046	1.45	1.66
UNIQUAC	145.6445	414.8008	0.06	0.0046	1.45	1.73
1,3-Dioxolane (1) + 1-chlorobutane (2) at 101.3 kPa						
Margules	0.3378	0.4871	0.11	0.0037	1.40	1.63
Van Laar	0.3487	0.4949	0.12	0.0037	1.40	1.64
Wilson	888.5569	554.1769	0.12	0.0036	1.42	1.64
NRTL	2301.8022	−808.1279	0.11	0.0037	1.41	1.63
UNIQUAC	23.7737	546.6873	0.11	0.0036	1.41	1.64
1,3-Dioxolane (1) + 2-chlorobutane (2) at 40.0 kPa						
Margules	0.4624	0.5651	0.18	0.0025	1.59	1.76
Van Laar	0.4662	0.5699	0.18	0.0026	1.59	1.77
Wilson	1251.7616	283.1565	0.19	0.0029	1.60	1.77
NRTL	1723.1248	−199.4811	0.19	0.0029	1.59	1.76
UNIQUAC	−173.7662	839.9905	0.19	0.0029	1.59	1.76
1,3-Dioxolane (1) + 2-chlorobutane (2) at 101.3 kPa						
Margules	0.4067	0.5098	0.14	0.0032	1.50	1.66
Van Laar	0.4134	0.5122	0.14	0.0032	1.51	1.67
Wilson	1245.2933	238.0096	0.14	0.0035	1.51	1.67
NRTL	1835.1145	−347.0372	0.14	0.0034	1.51	1.66
UNIQUAC	−194.0903	844.5504	0.14	0.0034	1.51	1.67

(*continued*)

TABLE VII Continued

1,3-Dioxolane (1) + 1-chloro-2-methylpropane (2) at 40.0 kPa						
Margules	0.4245	0.5676	0.11	0.0027	1.53	1.76
Van Laar	0.4342	0.5701	0.11	0.0028	1.54	1.77
Wilson	1051.6367	480.4404	0.11	0.0029	1.49	1.69
NRTL	2015.5572	−469.5749	0.11	0.0028	1.50	1.69
UNIQUAC	22.9590	602.2255	0.11	0.0028	1.48	1.69
1,3-Dioxolane (1) + 1-chloro-2-methylpropane (2) at 101.3 kPa						
Margules	0.3891	0.4467	0.27	0.0053	1.48	1.56
Van Laar	0.3922	0.4464	0.27	0.0053	1.48	1.56
Wilson	1396.5892	−98.8980	0.27	0.0053	1.48	1.56
NRTL	1352.8069	−64.3081	0.27	0.0053	1.48	1.56
UNIQUAC	−348.3529	983.6728	0.27	0.0053	1.48	1.56
1,3-Dioxolane (1) + 2-chloro-2-methylpropane (2) at 101.3 kPa						
Margules	0.4089	0.5269	0.15	0.0051	1.51	1.69
Van Laar	0.4190	0.5289	0.15	0.0051	1.52	1.70
Wilson	1162.6974	373.3730	0.16	0.0060	1.53	1.70
NRTL	2134.5351	−574.7263	0.16	0.0058	1.51	1.69
UNIQUAC	−121.2535	732.7617	0.16	0.0059	1.52	1.69

TABLE VIII Composition, $x_{1(az)}$ and boiling temperature, $T_{(az)}$ of azeotropic mixtures

System	P (kPa)	$x_{1(az)}$	$T_{(az)}$ (K)
1,3-Dioxolane +			
1-Chlorobutane	40.0	0.592	320.7
	101.3	0.643	346.5
2-Chlorobutane	40.0	0.136	314.0
	101.3	0.234	340.6
1-Chloro-2-methylpropane	40.0	0.171	315.0
	101.3	0.244	341.4

The systems present positive deviations from ideality and all of them, excepting 1,3-dioxolane + 2-chloro-2-methylpropane, present azeotropes, whose values of composition and temperature are listed in Table VIII.

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References

[1] I. Gascón, M. Domínguez, P. Cea, M.C. López and F.J. Royo (2001). *Chem. Thermodyn.*, **33**, 1361.
[2] H. Artigas, C. Lafuente, M.C. López, F. Royo and J.S. Urieta (1994). *J. Chem. Eng. Data*, **39**, 729.
[3] P. Cea, C. Lafuente, M.L. Sanz, F. Royo and J.S. Urieta (1995). *J. Chem. Eng. Data*, **40**, 692.
[4] H.C. Van Ness, S.M. Byer and R.E. Gibbs (1973). *AIChE. J.*, **19**, 238.
[5] M. Margules (1985). *Sitzunsber. Akad. Wiss. Wien, Math. -Naturwis. KI. II.*, **104**, 1234.
[6] J.J. Van Laar (1910). *Z. Phys. Chem.*, **72**, 723.
[7] G.M. Wilson (1964). *J. Am. Chem. Soc.*, **86**, 127.
[8] H. Renon and J.M. Praunsnitz (1968). *AIChE. J.*, **14**, 135.
[9] D.S. Abrams and J.M. Praunsnitz (1975). *AIChE. J.*, **21**, 116.
[10] J.A. Riddick, W.B. Bunger and T.K. Sakano (1986). *Organic Solvents. Physical Properties and Methods of Purification*, 4th Edn. Wiley Interscience, New York.

[11] P. Brocos, E. Calvo, A. Amigo, R. Bravo, M. Pinto, A.H. Roux and G.J. Roux-Desgranges (1998). *Chem. Eng. Data.*, **43**, 112.
[12] H. Artigas, C. Lafuente, M.C. López, F.M. Royo and J.S. Urieta (1997). *Fluid Phase Equilibria.*, **134**, 163.
[13] H.S. Wu and S.Y. Sandler (1989). *J. Chem. Eng. Data.*, **34**, 209.
[14] J. Gmehling and U. Onken (1981). *Dechema Chemestry Data Series*. Frankfurt/Main.
[15] L.C. Yen and S.S. Woods (1968). *AIChE. J.*, **14**, 95.
[16] A. Fredeslund, J. Gmehling and P. Radmussen (1977). Vapour–liquid Equilibria Using UNIFAC, pp. 68–74. Elsevier, Amsterdam.
[17] N. Silverman and D.P. Tassios (1984). *Ind. Eng. Chem. Process. Des. Dev.*, **23**, 586.
[18] J.A. Nelder and R.A. Mead (1965). *Comput. J.*, **7**, 308.