

Supporting information

Isothermal Vapor+Liquid Equilibrium and Thermophysical Properties for 1-Butyl-3-methylimidazolium Bromide + 1-Butanol Binary System

Mariana Teodorescu*

"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Splaiul Independentei 202, 060021 Bucharest, Romania

A. Equations applied which are not shown in the paper:

1. Equations for the mixtures density predictions from mixture refractive indices and refractive indices and densities of the pure components:

- Lorentz-Lorenz mixing rule: $\frac{n_D^2 - 1}{n_D^2 + 2} = \phi_1 \left(\frac{n_{D,1}^2 - 1}{n_{D,1}^2 + 2} \right) + \phi_2 \left(\frac{n_{D,2}^2 - 1}{n_{D,2}^2 + 2} \right)$ (S1)

- Gladstone-Dale mixing rule: $n_D - 1 = \phi_1 (n_{D,1} - 1) + \phi_2 (n_{D,2} - 1)$ (S2)

- Edwards mixing rule: $\frac{n_D - 1}{n_D} = \phi_1 \frac{n_{D,1} - 1}{n_{D,1}} + \phi_2 \frac{n_{D,2} - 1}{n_{D,2}}$ (S3)

- Eykman mixing rule: $\frac{n_D^2 - 1}{n_D + 0.4} = \phi_1 \frac{n_{D,1}^2 - 1}{n_{D,1} + 0.4} + \phi_2 \frac{n_{D,2}^2 - 1}{n_{D,2} + 0.4}$ (S4)

with $\phi_i = w_i \rho / \rho_i$ and $w_i = m_i / (m_1 + m_2)$, $i = 1, 2$ (components of the binary mixture: [bmim]Br (1) + 1-butanol (2))

2. Equation for surface tension deviation calculation:

$$\sigma^E = \sigma - x\sigma_1 - (1-x)\sigma_2 \quad (S5)$$

3. Equation for relative permittivity at optical frequency calculation:

$$\epsilon_r = n_D^2 \quad (S6)$$

4. Equation for dielectric permittivity calculation:

$$\epsilon = \epsilon_r \epsilon_0 \quad (S7)$$

where ϵ_0 is vacuum permittivity $\epsilon_0 = 8.8541878176.. \times 10^{-12}$ F/m

5. Equation for dielectric permittivity deviation calculation:

* Corresponding details: Tel: +40 213167912; Fax: +40 213121147;

E-mail address: mateodorescu@chimfiz.icf.ro

$$\varepsilon^E = \varepsilon - x\varepsilon_1 - (1-x)\varepsilon_2 \quad (\text{S8})$$

B. Tables which are not shown in the paper:

Table S1. Vapor+liquid equilibrium data for the [bmim]Br (1) + 1-butanol (2) system. Pressure, P_e , temperature, T , and [bmim]Br liquid phase composition, x_e , are experimental data and [bmim]Br vapor phase composition, y_c , activity coefficients, γ_1 , γ_2 , and excess Gibbs energy, G^E , are calculated data with Wilson model assuming real behavior of the vapor phase

x_e^a	y_c^a	P_e^b / kPa	γ_1	γ_2	G^E / (J mol ⁻¹)
$T^c = 353.15 \text{ K}$					
0	0	21.24	30.38	1	0
0.064	0.025	20.99	11.97	1.03	539
0.140	0.031	20.61	6.57	1.10	1010
0.215	0.033	20.61	4.48	1.19	1351
0.316	0.034	20.32	3.12	1.36	1666
$T^c = 363.15 \text{ K}$					
0	0	33.85	16.56	1	0
0.063	0.022	33.03	9.35	1.02	478
0.140	0.032	32.11	5.86	1.07	930
0.219	0.036	31.66	4.17	1.15	1281
0.321	0.038	31.03	3.00	1.30	1605
$T^c = 373.15 \text{ K}$					
0	0	51.69	15.04	1	0
0.065	0.024	50.38	8.82	1.02	485
0.140	0.035	49.01	5.73	1.07	932
0.224	0.040	48.09	4.04	1.15	1311
0.308	0.042	47.27	3.08	1.27	1590

^a $u_{xI} = 0.001$, ^b $u_P = 0.1\%$ of measured value, and ^c $u_T = 0.1 \text{ K}$.

Table S2. Parameters of the Wilson model, $\lambda_{12}-\lambda_{11}$ and $\lambda_{21}-\lambda_{22}$, and standard deviations for the pressure σ_p for the [bmim]Br (1) + 1-butanol (2) system, obtained from the correlation of the VLE data

T/K	$\lambda_{12}-\lambda_{11}/$ (J mol ⁻¹)	$\lambda_{21}-\lambda_{22}/$ (J mol ⁻¹)	σ_p/kPa
353.15	5325.301	27250.05	0.10
363.15	3650.401	44733.61	0.09
373.15	3459.938	46614.48	0.07

Table S3. Experimental refractive indexes, n_D , and their deviations from ideality, n_D^E , vs. mole fraction of [bmim]Br x , for [bmim]Br (1) + 1-butanol (2) binary system

x^a	n_D^b	n_D^E ^c	x^a	n_D^b	n_D^E ^c
^d $T = 298.15 \text{ K}$					
0	1.3973	0	0.584	1.4979	0.0200
0.094	1.4203	0.0100	0.667	1.5070	0.0176

0.193	1.4404	0.0165	0.779	1.5179	0.0132
0.271	1.4549	0.0203	0.818	1.5210	0.0108
0.345	1.4663	0.0214	1	1.5353	0
0.466	1.4834	0.0218	^d T = 308.15 K		
0	1.3932	0	0.584	1.4949	0.0203
0.094	1.4166	0.0103	0.667	1.5040	0.0178
0.193	1.4369	0.0168	0.779	1.5149	0.0132
0.271	1.4515	0.0206	0.818	1.5181	0.0109
0.345	1.4630	0.0217	1	1.5326	0
0.466	1.4803	0.0221			

^au_x = 0.001, ^bu_{nD} = 0.0001, ^cu_{n_D^E} = 0.0002, and ^du_T = 0.01 K.

Table S4. Redlich-Kister coefficients a_j [eq. (1)] and the standard deviations of the [bmim]Br composition σ_x and of the refractive index deviation $\sigma_{n_D^E}$ for [bmim]Br (1) + 1-butanol (2) binary system

T / K	a_0	a_1	a_2	σ_x	$\sigma_{n_D^E} \cdot 10^4$
298.15	0.0864	0.0266	0.0120	0.001	2.0
308.15	0.0875	0.0275	0.0123	0.001	1.9