Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A Methodology to Parameterize SAFT-type Equations of State for Solid Precursors of Deep Eutectic Solvents: The Example of Cholinium Chloride

Emanuel A. Crespo,[a] Liliana P. Silva,[a] Joel O. Lloret,[b] Pedro J. Carvalho,[a] Lourdes F. Vega,[c] Fèlix Llovell,[b*] and João A. P. Coutinho,[a]*

[a]CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;

[b]Department of Chemical Engineering and Materials Science, IQS School of Engineering, Universitat Ramon Llull, Via Augusta, 390, 08017 Barcelona, Spain

[c]Research and Innovation Center on CO_2 and H_2 (RICH), Center for Catalysis and Separation (CeCaS), Gas Research Center and Chemical Engineering Department. Khalifa University. PO Box 127788, Abu Dhabi, UAE

*Corresponding authors: felix.llovell@iqs.url.edu, Phone: +34 932670000

jcoutinho@ua.pt, Phone: +351 234401507 Fax: +351 234370084

VLE measurements

Table S1. Experimental VLE data and activity coefficients for [Ch]Cl (1) + EG (2) at temperature T, ethylene glycol molar composition x_2 and pressure p.

x_2	T / K	γ_2	x_2	T / K	γ_2
			P /MPa		
	0.10			0.07	
0.695	487.57	0.866	0.724	474.73	0.838
0.721	486.36	0.863	0.740	473.70	0.844
0.740	485.45	0.863	0.750	472.98	0.849
0.758	484.43	0.868	0.762	471.17	0.883
0.772	482.25	0.905	0.775	470.67	0.883
0.783	482.79	0.877	0.783	470.13	0.891
0.800	480.90	0.908	0.787	469.75	0.892
0.824	478.94	0.930	0.792	468.62	0.920
0.847	476.38	0.973	0.792	468.45	0.926
0.854	476.00	0.977	0.801	468.30	0.918
0.860	476.26	0.960	0.824	467.22	0.921
0.882	474.93	0.977	0.825	467.39	0.917
0.892	473.60	1.001	0.828	466.25	0.944
0.903	472.99	1.010	0.848	464.64	0.968
0.929	471.70	1.017	0.855	464.90	0.951
0.934	471.29	1.026	0.862	463.75	0.978
0.958	470.68	1.017	0.864	463.41	0.989
0.978	469.46	1.036	0.908	461.65	0.991
1.000	469.33	1.014	0.935	459.11	1.047
			0.952	458.31	1.054
			0.975	457.46	1.060
			1.000	457.28	1.036

[1]Standard uncertainties, u, are $u(x)$=0.001; $u(T)$=1 K and $u_r(p)$=0.005.

Energies and volumes of association for the [Ch]Cl + EG mixture

In **Tables S2-S3**, the values on orange, blue and red colors were transferred from previous works dealing with the modelling of symmetrical tetraalkylammonium halides, alkan-1-ols, and glycols, respectively. The values on grey are those obtained using the empirical approach proposed in this work (given in **eqs. 6-7**) while those on white are predicted using the combining rules (**eqs. 4-5**) or zero for forbidden interactions.

Table S2. Association energy matrix for the [Ch]Cl + EG mixture.

	Cation	Anion	O	H	CH	O'	H'
Cation	0	3384	0	0	0	3852	0
Anion	3384	0	0	3417	1692	0	3852
O	0	0	0	3450	1725	0	3889
H	0	3417	3450	0	0	3889	0
CH	0	1692	1725	0	0	0	0
O'	3852	0	0	3889	0	0	4384
H'	0	3852	3889	0	0	4384	0

Table S3. Association volume matrix for the [Ch]Cl + EG mixture.

	Cation	Anion	O	H	CH	O'	H'
Cation	0	2100	0	0	0	3028	0
Anion	2100	0	0	2174	2100	0	3028
O	0	0	0	2250	2250	0	3122
H	0	2174	2250	0	0	3122	0
CH	0	2100	2250	0	0	0	0
O'	3028	0	0	3122	0	0	4195
H'	0	3028	3122	0	0	4195	0

Fitting of pure-component parameters to pure fluid VLE data

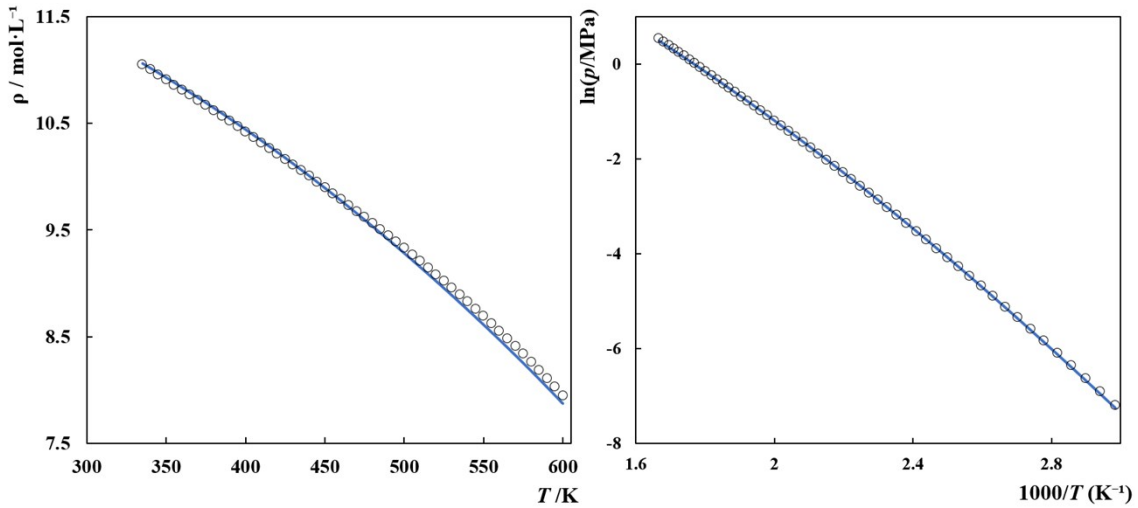

Figure S1. Saturated liquid densities and vapor pressures of phenol. Symbols represent experimental data form the DIPPR database[1] while the solid lines depict the soft-SAFT fitting to the data.

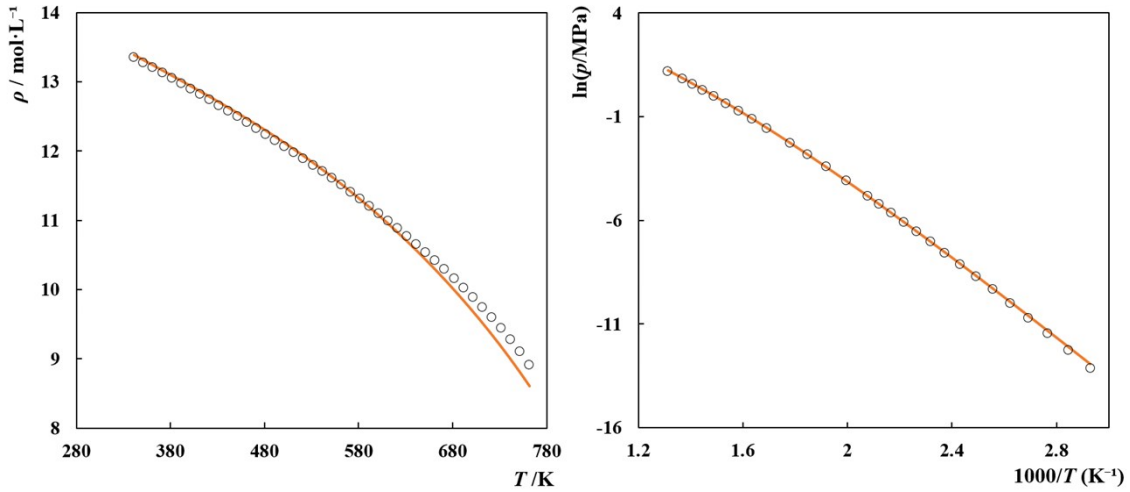

Figure S2. Saturated liquid densities and vapor pressures of glycerol. Symbols represent experimental data form the DIPPR database[1] while the solid lines depict the soft-SAFT fitting to the data.

References

(1) Daubert, T. E.; Sibul, H. M.; Stebbins, C. C.; Danner, R. P.; Rowley, R. L.; Adams, M. E.; Wilding, W. V; Marshall, T. L. *Physical and Thermodynamic Properties of Pure Chemicals: DIPPR: Data Compilation: Core + Supplements 1-10*; Taylor & Francis, 2000.