

## Accepted Manuscript

Experimental densities of 2,2,2-trifluoroethanol with 1-butyl-3-methylimidazolium hexafluorophosphate at high pressures and modelling with PC-SAFT

Moisés R. Currás, Marta M. Mato, Pablo B. Sánchez, Josefa García

PII: S0021-9614(17)30167-2  
DOI: <http://dx.doi.org/10.1016/j.jct.2017.05.029>  
Reference: YJCHT 5083

To appear in: *J. Chem. Thermodynamics*

Received Date: 20 July 2016  
Revised Date: 28 April 2017  
Accepted Date: 23 May 2017

Please cite this article as: M.R. Currás, M.M. Mato, P.B. Sánchez, J. García, Experimental densities of 2,2,2-trifluoroethanol with 1-butyl-3-methylimidazolium hexafluorophosphate at high pressures and modelling with PC-SAFT, *J. Chem. Thermodynamics* (2017), doi: <http://dx.doi.org/10.1016/j.jct.2017.05.029>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Experimental densities of 2,2,2-trifluoroethanol with 1-butyl-3-methylimidazolium hexafluorophosphate at high pressures and modelling with PC-SAFT

Moisés R. Currás, Marta M. Mato, Pablo B. Sánchez, Josefa García \*

*Department of Applied Physics, University of Vigo, 36310 Vigo, Spain*

---

## HIGHLIGHTS

- Density measurements at high pressures of TFE + [C<sub>1</sub>C<sub>4</sub>Im][PF<sub>6</sub>].
- Excess molar volumes have a sigmoid shape.
- Apparent molar volumes of IL indicating hydrogen bonding inexistent or scarce.
- PC-SAFT density correlations of 0.3 % for [C<sub>1</sub>C<sub>4</sub>Im][PF<sub>6</sub>] were obtained.
- An *ARD* of 3.1 % was achieved for PC-SAFT predictions of density for the mixtures.

---

## ABSTRACT

New data of densities at temperatures in the 288.15-333.15 K range and several pressures, up to 40 MPa, have been measured for 2,2,2-trifluoroethanol + 1-butyl-3-methylimidazolium hexafluorophosphate system using a vibrating tube densimeter. The combined expanded uncertainty at the 0.95 confidence level in the density measurements is 2 kg·m<sup>-3</sup>. Excess molar volumes,  $V_m^E$ , and apparent molar volumes,  $V_\phi$ , were determined from the density values of the pure compounds and mixtures. The influence of the temperature, pressure and composition on  $V_m^E$ ,  $V_\phi$ , was studied. In general, the dependence of  $V_m^E$  with the mole fraction is sigmoid showing that there is a competition between the breaking and formation of interactions and the packing effect;  $V_\phi$  was represented using the Redlich-Mayer equation, indicating that hydrogen bonding interactions are inexistent or scarce. Derived properties,  $\kappa_T$  and  $\alpha_p$  were calculated from the analytical differentiation of the Tait equation, and it was observed that the variation with pressure and temperature is very small for 1-butyl-3-methylimidazolium hexafluorophosphate. In addition, PC-SAFT parameters of 1-butyl-3-methylimidazolium hexafluorophosphate were optimized using density data at

Download English Version:

<https://daneshyari.com/en/article/4907231>

Download Persian Version:

<https://daneshyari.com/article/4907231>

[Daneshyari.com](https://daneshyari.com)