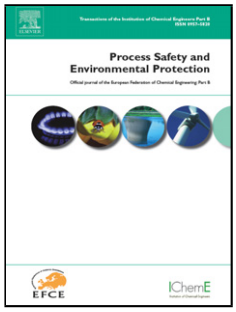

Title: A novel method for predicting melting point of ionic liquids

Authors: Mohammad Hossein Keshavarz, Hamid Reza Pouretedal, Ehsan Saberi

PII: S0957-5820(18)30047-8
DOI: https://doi.org/10.1016/j.psep.2018.02.015
Reference: PSEP 1301

To appear in: *Process Safety and Environment Protection*

Received date: 1-2-2017
Revised date: 20-8-2017
Accepted date: 22-2-2018

Please cite this article as: Keshavarz, Mohammad Hossein, Pouretedal, Hamid Reza, Saberi, Ehsan, A novel method for predicting melting point of ionic liquids.Process Safety and Environment Protection https://doi.org/10.1016/j.psep.2018.02.015

A novel method for predicting melting point of ionic liquids

Mohammad Hossein Keshavarz*, Hamid Reza Pouretedal and Ehsan Saberi

Department of Chemistry, Malek-ashtar University of Technology, Shahin-shahr, P.O. Box 83145/115, Islamic Republic of Iran

*To whom correspondence should be addressed

Tel: (0098) 0312 522 5071; *Fax: (0098) 0312 5225068; e-mail:* mhkeshavarz@mut-es.ac.ir; keshavarz7@gmail.com

Abstract

For industrial applications, it is important to know phase transition properties such as melting points of ionic liquids (ILs). A novel correlation is introduced to predict melting points of important classes of ILs including imidazolium-, pyridinium-, pyrrolidinium-, ammonium-, phosphonium-, and piperidinium-based ILs and different type of anions with specific cation/anion moieties. It is based only on the number of some of atoms in cationic and anionic structures as well as two correcting functions for the presence of some specific cation/anion moieties. The numbers of carbon, hydrogen and nitrogen atoms are used for cation. Meanwhile, the numbers of hydrogen, nitrogen, bromine, chlorine and aluminum atoms are applied for anion. The measured data of 195 different types of ILs were used to derive the new correlations. The calculated