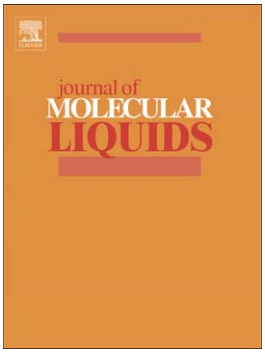

Prediction of heat capacities of ionic liquids using chemical structure based networks

Ali Barati-Harooni, Adel Najafi-Marghmaleki, Amir H Mohammadi

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Prediction of Heat Capacities of Ionic Liquids Using Chemical Structure based Networks

Ali Barati-Harooni,[a1] Adel Najafi-Marghmaleki,[a] Amir H Mohammadi[b,c,d 2]

[a] *Young Researchers and Elite Club, Ahvaz Branch, Islamic Azad University, Ahvaz, Iran*
[b] *Discipline of Chemical Engineering, School of Engineering, University of KwaZulu-Natal, Howard College Campus, King George V Avenue, Durban 4041, South Africa*
[c] *Institut de Recherche en Génie Chimique et Pétrolier (IRGCP), Paris Cedex, France*
[d] *Département de Génie des Mines, de la Métallurgie et des Matériaux, Faculté des Sciences et de Génie, Université Laval, Québec, QC G1V 0A6, Canada*

Abstract - Ionic liquids (ILs) have various desired properties which bring them as useful and applicable compounds in different industrial processes. Heat capacity of ILs is one of the main properties of them which is required in various engineering and design applications. Hence, developing accurate and general models for prediction of this property is important. In this communication, two accurate and general models based on radial basis function neural network (RBF-NN) and multilayer perceptron neural network (MLP-NN) were developed for estimation of heat capacities of ILs. The input parameters of the models are temperature, molecular weight of IL and several structural related parameters for each IL. The models were developed based on 2940 experimental data for 56 ILs. The reliability and accuracy of predictions of the developed models were examined by using statistical and graphical methods as well as comparing the results of the models with outcomes of recently developed literature correlations. Results show that the developed models are accurate and reliable and are superior to literature correlations for

Corresponding author:
[1]1. Email Address: alibarati.2012@yahoo.com (**A. Barati-Harooni**)

[2]2. Email Address: a.h.m@irgcp.fr and amir_h_mohammadi@yahoo.com (**A. H. Mohammadi**)