Accepted Manuscript

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PII: S0167-7322(16)32695-2

DOI: doi: 10.1016/j.molliq.2016.11.119

Reference: MOLLIQ 6666

To appear in: Journal of Molecular Liquids

Received date: 11 September 2016 Revised date: 20 October 2016 Accepted date: 27 November 2016



Please cite this article as: Ali Barati-Harooni, Adel Najafi-Marghmaleki, Amir H Mohammadi, Prediction of heat capacities of ionic liquids using chemical structure based networks, *Journal of Molecular Liquids* (2016), doi: 10.1016/j.molliq.2016.11.119

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ACCEPTED MANUSCRIPT

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

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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

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