

Accepted Manuscript

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PII: S0167-7322(17)30678-5
DOI: doi: [10.1016/j.molliq.2017.05.095](https://doi.org/10.1016/j.molliq.2017.05.095)
Reference: MOLLIQ 7387

To appear in: *Journal of Molecular Liquids*

Received date: 14 February 2017
Revised date: 15 May 2017
Accepted date: 21 May 2017



Please cite this article as: Juan A. Lazzús, Geraldo Pulgar-Villarroel, Fernando Cuturrufo, Pedro Vega, Development of a group contribution method for estimating surface tension of ionic liquids over a wide range of temperatures, *Journal of Molecular Liquids* (2017), doi: [10.1016/j.molliq.2017.05.095](https://doi.org/10.1016/j.molliq.2017.05.095)

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Development of a group contribution method for
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range of temperatures

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Abstract

A group contribution methods for estimating the surface tension of ionic liquids as a function of the absolute temperature, is presented. A total of 2286 experimental data points from 226 data sets of 154 ionic liquids were collected from the specialized literature. This database covers a temperature range of 263–533 K and a surface tension range of 0.015–0.062 N·m⁻¹, for a heterogeneous set of ionic liquid-types such as imidazolium, ammonium, phosphonium, pyridinium, pyrrolidinium, and piperidinium. A correlation set containing the 75% of the overall database was used in order to calculate the contribution values of 10 structural cation groups and 30 structural anion groups. Then, a prediction set containing the other 25% of the overall database with data sets not used in the correlation phase was used in order to test the capabilities and accuracy of the proposed method. The results show that the proposed method can estimate the surface tension of several ionic liquids with a better accuracy than other methods available in the literature, with an average absolute relative deviation of 2.8% and a correlation coefficient of 0.98.

Keywords: Ionic liquids, Surface tension, Group contribution method, Genetic algorithm, Parameter estimation.

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