Thermophysical Properties of Ionic Liquids - ILThermo Archival Database: 3. Engineering Applications

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Critically evaluated experimental data are essential to carry out innovative chemical process design, or to improve material and energy efficiencies of existing chemical processes. Developed under the auspices of IUPAC (Project 2003-020-2-100), *ILThermo* (http://ilthermo.boulder.nist.gov/) is a data archive of experimental thermophysical properties (including 120 thermodynamic, transport and thermochemical properties) of ionic liquids and mixtures that contain them. Version 1.0 was announced at COIL-1 [1]. Detailed capabilities have been described [2]. Recently, Version 2.0 [3] was released by NIST's Thermodynamics Research Center. *ILThermo* is a web-based open-access database that provides data and metadata from published experimental studies of ionic liquids, including numerical values of thermophysical properties, chemical structures, measurement methods, sample purity, critically evaluated standard uncertainties of property values, as well as other significant measurement details. Version 2.0 is keyed on chemical structure of each chemical species that is curated, which brings inherent advantages to users of the database. Best practices are described for search and retrieval of thermophysical properties and phase behavior data from *ILThermo* for use in engineering applications.

References:

 J. W. Magee, J. A. Widegren, M. Frenkel, Q. Dong, C. Muzny, R. D. Chirico and V. V. Diky "Comprehensive Data Retrieval System for Ionic Liquids," 1st International Congress on Ionic Liquids, Salzburg, Austria, June 19-22, 2005.
Q. Dong, C. D. Muzny, A. Kazakov, V. Diky, J. W. Magee, J. A. Widegren, R. D. Chirico, K. N. Marsh, and M. Frenkel, J. Chem. Eng. Data, 2007, 52, 1151-1159.

[3] A. Kazakov, J.W. Magee, R.D. Chirico, V. Diky, C.D. Muzny, K. Kroenlein and M. Frenkel "NIST Standard Reference Database 147: NIST Ionic Liquids Database - (*ILThermo*)", Version 2.0, National Institute of Standards and Technology, Gaithersburg MD, 20899, http://ilthermo.boulder.nist.gov.