

Ionic Liquids in the Dortmund Data Bank

Ionic liquids have become very popular in the last years. They are discussed as "designer solvents" for the use in chemical reactions (e. g. biphasic reactions), as selective solvent for separation processes (extraction, extractive distillation, absorption, etc.), in electrochemistry, etc.

For the development of new processes using ionic liquids besides the various pure component properties (viscosity, density, heat capacity, melting point, etc.) in particular the knowledge of the phase equilibrium behavior as function of temperature, i. e. activity coefficients at infinite dilution, vapor-liquid equilibria, liquid-liquid equilibria, solid-liquid equilibria, excess enthalpies, ... is required. A few years ago nearly no data were available. But during the last years different research groups started to measure the required pure component properties and mixture data. A great part of this data are not available up to now from literature.

Unpublished data from the industrial chemistry research group of Prof. Gmehling and other sources (private communications) as well as published data are continuously stored in special files of the Dortmund Data Bank. At the moment these files already contain the following amount of data (pure component data, mixture data) for more than 400 different ionic liquids:

Data Bank	Data Sets	Data Points
Activity coefficients at infinite dilution in ionic liquids	6448	6448
Activity coefficients at infinite dilution in ionic liquids and additional solvent	95	204
Vapor-liquid equilibria (binary and ternary VLE)	884	9782
Vapor-liquid equilibria (electrolyte containing systems)	125	1639
Gas solubilities (GLE)	483	1502
Solid-liquid equilibria (SLE)	188	2878
Liquid-liquid equilibria (LLE)	663	6041
Excess enthalpies (HE)	103	1114
Densities, volumes, excess volumes	547	5772
...
Pure component properties	1715	15999
Sum	11292	51876 February 2009

447 publicly available sources (mainly scientific articles) have been evaluated but a significant percentage of the data is not available from literature up till now.

If the use of ionic liquids for a specific application is planned (e. g. as solvent for chemical reactions, selective entrainer for the various separation processes – extractive distillation, extraction, absorption or other applications) these data are extremely helpful.

The above mentioned data bank for ionic liquids for internal use within your company is available for a price of 4200 € in form of ASCII-files. However, for the efficient use of these data we would

recommend the use of a software package, which is available for 2100 €. This software package allows to retrieve the data using several search options (components, systems, literature), has graphical data representation, has copy and print capabilities, and allows data export to PPDx and Aspen INP files. Furthermore with the help of the software package the user can define new components or store his own experimental data. At the same time with the software package the required basic data for all the compounds used, such as name, formula, CAS registry number, Antoine constants with the range of validity, critical data, acentric factor, density, van der Waals properties, heat of fusion, melting point, dipole moment, etc. are delivered.

If you are interested in the data for ionic liquids please do not hesitate to get in touch with Prof. Gmehling directly or with DDBST.

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