

**DDBST**DORTMUND DATA BANK
SOFTWARE & SEPARATION
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DDB 2018 - Ionic Liquids

Ionic Liquids in the Dortmund Data Bank

Ionic liquids have become very popular in the last years, because of their unique properties, e.g. extremely low vapor pressure, wide electrochemical window, and promising selectivity/capacity. Therefore, they are discussed as "designer solvents" for the use in

- chemical reactions (e. g. biphasic reactions)
- as selective solvent for separation processes (extraction, absorption,)
- electrochemistry, etc.

For the development of new processes using ionic liquids besides the various pure component properties like

- viscosity
- density
- heat capacity
- heat of fusion
- melting point
- heat of transition
- thermal conductivity
- surface tension
- speed of sound
- electrical conductivity

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 (miscibility gaps)
- solid-liquid equilibria (melting points of mixtures)
- gas solubilities
- salt solubilities
- excess enthalpies
- excess heat capacities

with ionic liquids is required.

A few years ago nearly no data were available for systems with ionic liquids. But during the last years different research groups started to measure the required pure component properties and mixture data.

Published as well as unpublished data (private communications) are continuously stored in the Dortmund Data Bank (DDB). At the moment DDB contains pure component and mixture data for 2,700 ionic liquids:

Data Bank	Data Sets	Data Points
Activity coefficients at infinite dilution in ionic liquids	47,000	47,000
Vapor-liquid equilibria (binary and ternary VLE)	5,630	61,640
Gas solubilities (GLE)	1,820	8,530
Solid-liquid equilibria (SLE)	1,360	15,600
Liquid-liquid equilibria (LLE)	5,250	62,680
Excess enthalpies (HE)	360	5,940
Excess heat capacities (CPE)	620	7,930
Densities, volumes, excess volumes	4,780	54,090
Mixture viscosities	4,990	51,300
Mixture surface tensions	990	10,279
Mixture speed of sound	3,490	40,810
Electrical conductivity	2,650	30,380
...
Pure Component Properties	10,070	77,650
Total	96,800	535,660

For building the data bank for ionic liquids 6,130 publicly available sources (mainly scientific articles) have been evaluated. 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 extraction, absorption or other applications) these data are extremely helpful. The PC version of the data bank for ionic liquids is available for 19,000 €*. For the efficient use of the data, we recommend the use of a software package which is available for 4,800 € for a PC version*. This software package allows the data retrieval using several search options (components, systems, literature), has graphical data representations, copy and print capabilities, and allows data export to PPDX and Aspen™ INP files.

With the help of the software package new components can be defined and experimental data added to the data bank. At the same time the required basic data for the compounds, such as

- name and formula
- CAS registry number
- Antoine constants with the range of validity
- critical data and acentric factor
- density
- van der Waals properties
- melting point and heat of fusion
- dipole moment, etc.

are delivered. But because of the negligible vapor pressure, Antoine constants, critical data and acentric factors are available only for a limited number of ionic liquids.

* For universities a discount of 75% is available. Changes and errors are possible regarding all information.

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