

**DDBST**DORTMUND DATA BANK
SOFTWARE & SEPARATION
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DDB 2017 - 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, good thermal and chemical stability, 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, extractive distillation, 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 (heats of mixing)
- 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Published as well as unpublished data (private communications) are continuously stored in the Dortmund Data Bank. At the moment the data bank contains pure component and mixture data for 2,470 ionic liquids:

Data Bank	Data Sets	Data Points
Activity coefficients at infinite dilution in ionic liquids	41,300	41,300
Vapor-liquid equilibria (binary and ternary VLE)	5,000	53,800
Gas solubilities (GLE)	1,620	6,750
Solid-liquid equilibria (SLE)	1,270	14,400
Liquid-liquid equilibria (LLE)	4,770	57,000
Excess enthalpies (HE)	340	5,700
Excess heat capacities (CPE)	610	7,500
Densities, volumes, excess volumes	4,200	47,700
Mixture viscosities	3,700	38,700
Mixture surface tensions	840	8,900
Mixture speed of sound	2,330	28,300
Electrical conductivity	2,370	27,200
...
Pure Component Properties	9,000	68,900
Total	82,600	445,300

5,100 publically 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 data bank for ionic liquids is available for 4,650 € for a single workstation license. The added software package allows to retrieve the data using several search options (components, systems, literature), has graphical data representations, has copy and print capabilities, and allows data export to PPDx and Aspen™ INP file.

With the help of the software package the user can define new components or store his own experimental data. At the same time the required basic data for the compounds, such as

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

are delivered. Because of the negligible vapor pressure, Antoine constants, critical data and acentric factors are seldom available for ionic liquids.

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