

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Published as well as unpublished data (private communications) are continuously stored in the Dortmund Data Bank (DDB). The amount of ionic liquids related data stored in the DDB are given in the table.

| Data Bank   | Data Sets      | Data Points    |
|---|----------------|----------------|
| Activity coefficients at infinite dilution in ionic liquids | 65,500         | 65,500         |
| Vapor-liquid equilibria (binary and ternary VLE)            | 9,600          | 100,250        |
| Gas solubilities (GLE)                                      | 3,400          | 17,450         |
| Solid-liquid equilibria (SLE)                               | 2,450          | 23,800         |
| Liquid-liquid equilibria (LLE)                              | 7,700          | 96,250         |
| Excess enthalpies (HE)                                      | 440            | 6,750          |
| Excess heat capacities (CPE)                                | 800            | 10,900         |
| Densities, volumes, excess volumes                          | 7,200          | 79,900         |
| Mixture viscosities   | 10,550         | 104,000        |
| Mixture surface tensions                                    | 1,900          | 18,800         |
| Mixture speed of sound                                      | 7,950          | 86,050         |
| Electrical conductivity                                     | 6,000          | 71,500         |
| ...   | ...            | ...            |
| Pure Component Properties                                   | 15,900         | 117,850        |
| <b>Total</b>  | <b>148,750</b> | <b>864,300</b> |

For building the data bank for ionic liquids approx. 7,700 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. For the efficient use of the data, the DDB Access package is mandatory. 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.

Changes and errors are possible regarding all information and prices.