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DDBSP 2010 – Ionic Liquids

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.
- electrochemistry, etc.

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

- viscosity
- density
- heat capacity
- melting point
- heat of fusion
- heat of transition
- thermal conductivity
- surface tension
- speed of sound, 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 (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. But during the last years different research groups started to measure the required pure component properties and mixture data.
Unpublished data from the industrial chemistry research group of Prof.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 622 different ionic liquids:

	August 2009		September 2010	
Data Bank	**Data Sets**	**Data Points**	**Data Sets**	**Data Points**
Activity coefficients at infinite dilution in ionic liquids	7538	7538	9925	9925
Activity coefficients at infinite dilution in ionic liquids and additional solvent	95	204	95	204
Vapor-liquid equilibria (binary and ternary VLE)	1086	11587	1312	13968
Gas solubilities (GLE)	527	1646	620	2227
Solid-liquid equilibria (SLE)	228	3257	295	3854
Liquid-liquid equilibria (LLE)	804	7593	1000	9635
Excess enthalpies (HE)	121	1379	124	1420
Densities, volumes, excess volumes	708	7780	1209	13860
Mixture viscosities	-	-	221	3472
...	...	...	...	...
Pure component properties	2035	18692	2544	24353
Sum	**13357**	**62418**	**17824**	**85432**

673 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 above mentioned data bank for ionic liquids for internal use within your company is available for a price of 5700 € 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 representations, 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 the compounds used, such as

- name
- 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. Due to their negligible vapor pressure, properties like Antoine constants, critical data and acentric factor are available for normal organic components but not for the ionic liquids.