IUPAC Ionic Liquids Database
- ILThermo

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Outline

- Background Information
- ILThermo Database Organization
- Ionic Liquids Specification
- Web Presentation
What are Ionic Liquids (ILs) ?

- ILs are salts that melt below 100\(^0\)C, composed wholly of ions.
  - CATIONS such as substituted imidazoliums, substituted pyridiniums or others
  - ANIONS such as borates, phosphates and halides and others

- Naming examples and structures

\[
\begin{align*}
\text{CATION} & \quad \text{ANION} \\
(1) & \quad 1\text{-butyl-3-methylimidazolium hexafluorophosphate} \\
(2) & \quad N\text{-butylpyridinium tetrafluoroborate}
\end{align*}
\]
Why are ILs a Hot Topic?

- **The materials are unique (properties and variety)**
  - Tunability
  - Negligible vapor pressure
  - Good thermal stability
  - Wide liquid range
  - Electrolytic conductivity

- **The prospects for ILs applications are vast**
  - **Possibility to establish environmentally benign chemical processing**
    - 20 million ton VOCs discharged into atmosphere per year
    - 2/3 of all industrial emission and 1/3 of VOCs emission nationwide from traditional solvents
    - Global climate change, poor urban air quality, and human illness
  - **Potential to revolutionize the way how solvents are utilized**
    - New extraction, catalysis, separations, and polymer processes
    - New chemical synthesis
    - Enhancement of existing processes
  - **Opportunities to develop task-target performance chemicals**
    - Engineering fluids for machinery and equipment
    - New materials in the automotive, textile, construction, oil and gas, and energy industries
Dramatic Increase in Research on Ionic Liquids

Worldwide Escalation in Number of Ionic Liquids Publications (Web of Science)

<table>
<thead>
<tr>
<th>Year</th>
<th>Publications</th>
</tr>
</thead>
<tbody>
<tr>
<td>1990</td>
<td>3</td>
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</tr>
<tr>
<td>2004</td>
<td>786</td>
</tr>
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<td>Total</td>
<td>2421</td>
</tr>
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</table>
Workshops and Conferences

2000
NATO Advanced Research Workshop – “Green Industrial Applications of Ionic Liquids” in Heraklion, Crete, Greece with 41 participants

2001 – 2003

2002
Workshop on Ionic Liquids: Properties of Ionic Liquids and their Application in Chemical Engineering. IACT/IUPAC International Conference on Chemical Thermodynamics, Rostock, Germany

2003
Ionic Liquids Symposium, in Melbourne, Australia

2004
Ionic Liquids Workshop of Background, State-of-the-Art, and Academic/Industrial Applications in The University of Alabama, Tuscaloosa, AL

2005
1st International Congress on Ionic Liquids in Salzburg, Austria. More than 400 participants from 33 countries and six continents
**1st International Congress on Ionic Liquids**

**Overall:**
279 presentations

**Main Topics:**
- New ionic liquids – synthesis of ionic liquids
- Characterization and thermodynamic properties and modeling
- Toxicology, persistence and sustainability
- Interesting new applications in synthesis, catalysis, biocatalysis, separation, electrochemistry and analytics

**Thermodynamic Property Data:**
- 72 presentations
- 26% of total presentations

*Salzburg, Austria, June 2005*
**Message from the Salzburg Congress**

**Opportunities**

- Storage and delivery of hazardous gases like phosphine or BF₃
- Detect ethanol by using ILs as solvents for advanced NMR-techniques
- ILs based electrolytes for dye-sensitized solar-cells and for the deposition of metals
- Suitable solvents for the dimerization of olefins

**Challenges**

- Cost of ILs and ILs technology
- Complexity of coordination, speciation, and extraction in chemical processes when utilizing ILs
- Limited information and data on structural variations, chemical and physical properties, corrosion and toxicity.
"A public, free, independently verified, web-based database of physical, thermodynamic, and related data is urgently needed. There is also an immediate need for toxicity, biodegradation, bioaccumulation, and other safety, health, and environmental impact data. New analytical tools are also required for assessing the purity of ionic liquids. In addition, applications-oriented research on ionic liquids should include cost-benefit, economic, and life-cycle analyses."

Professor Robin D. Rogers
Center for Green Manufacturing
The University of Alabama
“Green Industrial Applications of Ionic Liquids”
NATO Advanced Research Workshop, April, 2000
Two IUPAC Task Groups on Ionic Liquids Data

  - Encourage systematic studies of thermodynamic and thermophysical properties
  - Recommend a reference ionic liquid and make reference quality measurements

  - Create a new database of experimental thermodynamic properties for ionic liquids
  - Provide a web-based comprehensive data retrieval system with free public access
IUPAC Ionic Liquids Database - ILThermo

- **Aim**
  - Provide users worldwide with an up-to-date collection of experimental investigations on ILs

- **Subject Coverage:**
  - Chemical identification of ions and ILs
  - Chemical systems of pure ILs, binary and ternary mixture systems containing ILs
  - Thermodynamic, thermochemical and transport properties
  - Phase behavior and solvent properties
  - Sample purity
  - Metadata (state variables, phases, system constraints, and measurement technology...)
  - Reviews and bibliography

- **Developments and Plans**
  - Develop and maintain at NIST as an ongoing commitment
  - Provide FREE public access
  - Anticipated public release for December of 2005
NIST-SOURCE for ILs Depository and Data Entry

Outside Contributors

Guided data entry

NIST-SOURCE data archive system

ILThermo

ILs

NIST-SOURCE

Depository of all experimental thermophysical and thermochemical properties reported in the world’s scientific literature

Include

✓ 2,200,000 numerical property values and their uncertainties
✓ 17,400 pure compounds
✓ 24,700 binary and ternary mixture systems
✓ 4,000 reaction systems
✓ data entry rate is near 300,000 values per year
ILThermo Database Organization

Group 1
- Bibliographic sources
- Ions

Group 2
- Ternary mixtures
- Binary mixtures
- Chemical (ionic) compounds

Group 3
- Source and purity of samples

Group 4
- Metadata – data used to describe numerical data (state variables, phases, constraints, measurement...)

Group 5
- Numerical property data sets
  - Constant values
  - One variable
  - Two variables
  - Three variables
Specifications for ILThermo Database

- Ions
- Ionic liquids
- Relation of ions and ionic liquids
- Pure ionic compounds
- Binary mixtures containing ionic liquids
- Ternary mixtures containing ionic liquids
- Measurement technology
- Sample purity
- Physiochemical property data
- Uncertainty
Identification of Ions

Each cation or anion is identified by:
- Chemical Abstract Registry number
- Ionic formula
  - the simplest ratio of cation and anion; not discrete entities
- Ionic charge
  - positive charge for cation and negative charge for anion
- Name
- Structure

Examples

Name: Hexafluorophosphate

CATION – CASRN: 80432-08-2 Formula: C$_8$H$_{15}$N$_2$ Charge: 1
Name: 1-Butyl-3-methylimidazolium
Identification of Ionic Liquid

AN IONIC COMPOUND is represented in the same way as other chemical substances.

- Chemical Abstract Registry number
- Molecular formula
- Molecular weight
- Name
- Molecular structure

Example

IONIC LIQUID – CASRN: 174501-64-5 Formula: C_8H_{15}F_6N_2P
Molecular weight: 284.18
Name: 1-butyl-3-methylimidazolium hexafluorophosphate

\[ \text{H}_3\text{C-}[\text{N}^+\text{CH}_3\text{CH}_3\text{CH}]-\text{CH}_3 \]

\[ \text{F-} \text{P} \rightarrow \text{F} \]

CATION – 80432-08-2, C8H15N2, 1-butyl-3-methylimidazolium
ANION – 16919-18-9, PF6, Hexafluorophosphate
Relation of Ions and Ionic Compounds

- For any selected cation or anion, there are links to all ionic compounds containing this ion.
- For any selected ionic compound, there are links to all ions constituting this ionic liquid.
Chemical Systems of Ionic Liquids

- **Pure ionic compounds**
  
  Cation + anion

- **Binary mixtures containing ionic liquids**
  
  Ionic liquid + molecular compound
  
  Molecular compounds: (a) water; (b) alcohols; (c) aliphatic alkanes; (d) cyclohydrocarbons; (e) aromatic hydrocarbons; (f) chloroalkanes; and (g) CO₂ and other gases
  
  **Examples:**
  - Solubility of oxygen and carbon dioxide in 1-butyl-3-methyl imidazolium tetrafluoroborate
  - Apparent molar volume and isentropic compressibility of ionic liquid 1-butyl-3-methylimidazolium bromide in water, methanol, and ethanol

- **Ternary mixtures containing ionic liquids**
  
  **Examples:**
  - Conductivities and viscosities of the ionic liquid [bmim][PF₆] + water + ethanol and [bmim][PF₆] + water + acetone
  - Ionic liquids/water distribution ratios of some polycyclic aromatic hydrocarbons
Sample Purity

1) **Original Source of the Sample**
   Standard reference sample; Commercial source; Synthesized by author; Isolated from a natural product; not stated

2) **Initial Purity of sample**
   Reported at a percentage of mole percent or mass percent; water and halid impurity identified

3) **Method of purification**
   21 common methods identified such as adsorption of impurities, crystallization, a chemical reagent, fractional distillation ...

4) **Final purity of sample**

5) **Method of Purity Analysis**
   13 methods identified such as chemical analysis, density, differential scanning calorimeter, mass spectrometry, NMR ...
**Physicochemical Property Data**

- **Data Type**
  
  Strict application of the Gibbs Phase Rule (GPR) forms the basis for organizing numerical data in the database. The number of independent variables, called degree of freedom of the system given by GPR, is a fundamental criteria used to classify all types of physicochemical properties as:
  
  - Constants (critical temperature and pressure)
  - with one state variable (heat capacity – Temperature $T$)
  - with two state variables (solubility – $T$, Composition $X$)
  - with three state variables (viscosity – $T$, $X$ and Pressure $P$)

- **Data Set**
  
  Each data set / data point in the database consists of two parts:
  
  - metadata (identification of chemical components, phases, units, constraints, chemical composition, state variables, measurement purpose and method …)
  - numerical data (values of state variables, property, and the estimated uncertainty)
“Estimates of uncertainty are the measure of data quality for all experimentally determined quantities and form the basis for the understanding, evaluation, and application of all scientific data.

... Although few scientists would disagree that the reporting of reliable uncertainty information is important, it is broadly recognized that the nature and extent of that reporting in the literature is highly variable”. 
Data Uncertainty (2)

1. Source and purity of sample
2. Measurement technique limits
3. Calibration of instruments
4. Care used to perform the measurement
5. Completeness and adequacy of description of procedure
6. Agreement among duplicate measurements, or between measurements on standard samples and other accepted values
7. Special effect such as contamination or decomposition of sample
8. Estimates of uncertainty, precision, or reproducibility given by the investigator
9. Experience and credibility of the investigator
Web Presentation of Physicochemical Property Data for Ionic Liquids

ILThermo Database
Main Menu
IUPAC Ionic Liquids Database

- (ILThermo)

IUPAC Ionic Liquids Database is an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structures, properties, and uses.

Property Data for Ionic Liquids

- Ions
- Ionic Liquids
- Property
- Literature

Property Data for Binary Mixtures Containing Ionic Liquids

- Ions
- Ionic Liquids
- Property
- Literature

Property Data for Ternary Mixtures Containing Ionic Liquids

- Ions
- Ionic Liquids
- Property
- Literature

Search Ions or Ionic Liquids

- Ions
- Ionic Liquids

About Search Methods
Search Criteria

Ions
CASRN
Formula
Charge
Names

Ionic Liquids
CASRN
Formula
Molecular weight
Names

Property
Category
Description

Bibliography
Author’s name
Journal title
Article title
Year of publication

To be added
Measurement method
Sample purity
Other statistics
How to Search A Piece of Data by Ions?

Reference:
Title: Thermochemistry of ionic liquid heat-transfer fluids
Authors: M. E. Van Valkenburg, R. L. Vaughn, M. Williams and J. S. Wilkes

Ionic liquid studied:
Name: 1-ethyl-3-methylimidazolium tetrafluoroborate
CASRN: 143314-16-3
Formula: C₆H₁₁BF₄N₂

Measurements of:
- Heat capacity at constant pressure
- Specific density
- Triple point temperature
- Thermal conductivity
- Viscosity
- Normal melting temperature
- Enthalpy of Transition

Total 16 property data sets
IUPAC Ionic Liquids Database - (ILThermo)

IUPAC Ionic Liquids Database is an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structures, properties, and uses.

Property Data for Ionic Liquids

<table>
<thead>
<tr>
<th>Ions</th>
<th>Ionic Liquids</th>
<th>Property</th>
<th>Literature</th>
</tr>
</thead>
</table>

Property Data for Binary Mixtures Containing Ionic Liquids

<table>
<thead>
<tr>
<th>Ions</th>
<th>Ionic Liquids</th>
<th>Property</th>
<th>Literature</th>
</tr>
</thead>
</table>

Property Data for Ternary Mixtures Containing Ionic Liquids

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<th>Ions</th>
<th>Ionic Liquids</th>
<th>Property</th>
<th>Literature</th>
</tr>
</thead>
</table>

Search Ions or Ionic Liquids

<table>
<thead>
<tr>
<th>Ions</th>
<th>Ionic Liquids</th>
</tr>
</thead>
</table>

About Search Methods

Copyright NIST 2005
### IUPAC Ionic Liquids Database

- **ILThermo**

**Available Cations or Anions:**

<table>
<thead>
<tr>
<th>CASRN</th>
<th>Formula</th>
<th>Ionic Charge</th>
<th>Ionic Names</th>
</tr>
</thead>
<tbody>
<tr>
<td>14874705</td>
<td>BF4</td>
<td>-1</td>
<td>Borate(1-), Tetrafluoroborate, Tetrafluoroborate, Tetrafluoroborate (BF4); Tetrafluoroborate anion; Tetrafluoroborate(1-);</td>
</tr>
<tr>
<td>24953679</td>
<td>Br</td>
<td>-1</td>
<td>Bromide; Bromide (Br-); Bromide ion; Bromide ion (Br1-); Bromide ion(1-); Bromide(1-); Bromine ion; Bromine ion(1-); Bromine(1-); Bromine, ion (Br1-); Hydrobromic acid, ion(1-);</td>
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<tr>
<td>98837980</td>
<td>C2F5NO4S2</td>
<td>-1</td>
<td>Bis(pentafluorosulfonyl)imide; Bis(trifluoromethylsulfonyl)imide; Methanesulfonamide, 1,1,1-trifluoro-1H-(trifluoromethyl)sulfonyl]-ion(1-);</td>
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<tr>
<td>37181398</td>
<td>CF3O3S</td>
<td>-1</td>
<td>Methanesulfonic acid, trifluoro-; triflate; Triflate anion; Triflate ion ([CF3SO3]-); Trifluoromethanesulfonate; Trifluoromethanesulfonate(1-); Trifluoromethanesulfonic acid ion(1-); Trifluoromethanesulfonic acid;</td>
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<tr>
<td>16887006</td>
<td>Cl</td>
<td>-1</td>
<td>chloride ion;</td>
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<tr>
<td>16919189</td>
<td>F5P</td>
<td>-1</td>
<td>Hexafluorophosphate; Hexafluorophosphate ion; Hexafluorophosphate(1-); Hexafluorophosphate(1-) ion; Phosphate(1-), hexafluoro-;</td>
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<tr>
<td>85100289</td>
<td>C10H19N2</td>
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<td>1-Hexyl-3-methylimidazolium; 3-Hexyl-1-methylimidazolium; 1-Himidazolium, 1-hexyl-3-methyl-;</td>
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<td>17863103</td>
<td>C12H23N2</td>
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<td>1H-imidazolium, 1-methyl-3-octyl-;</td>
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<tr>
<td>45428103</td>
<td>C16H13N2</td>
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<td>1H-imidazolium, 1-dodecyl-3-methyl-;</td>
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<td>45470324</td>
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<td>1,3-Dimethylimidazolium; 1H-imidazolium, 1,3-dimethyl-;</td>
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<td>13197159</td>
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<td>1,2-Dimethyl-3-ethylimidazolium; 1-Ethyl-2,3-dimethylimidazolium; 1H-imidazolium, 1-ethyl-2,3-dimethyl-;</td>
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<td>80432002</td>
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<td>1-Butyl-3-methylimidazolium; 1H-imidazolium, 1-butyl-3-methyl-;</td>
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<td>15731070</td>
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<td>1-Butyl-2,3-dimethylimidazolium; 1H-imidazolium, 1-butyl-2,3-dimethyl-; 3-Butyl-1,2-dimethylimidazolium;</td>
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### Ionic liquid(s) Containing the Ion - 14874705

<table>
<thead>
<tr>
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<th>Chemical Formula</th>
<th>Molec. Weight</th>
<th>Ionic Liquid Name</th>
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<tbody>
<tr>
<td></td>
<td>143314163</td>
<td>C3H11BF4N2</td>
<td>197.97</td>
<td>1-ethyl-3-methylimidazolium tetrafluoroborate; 1H-imidazolium, 1-ethyl-3-methyl-, tetrafluoroborate(1-); [EMIM][BF4].</td>
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<tr>
<td></td>
<td>174501656</td>
<td>C3H15BF4N2</td>
<td>226.03</td>
<td>1-butyl-3-methylimidazolium tetrafluoroborate; 1H-imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-); [BMIM][BF4].</td>
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<tr>
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<td>203389280</td>
<td>C3H14BF4N</td>
<td>223.02</td>
<td>N-butyl/pyridinium tetrafluoroborate; pyridinium, 1-butyl-, tetrafluoroborate(1-);</td>
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<tr>
<td></td>
<td>244193608</td>
<td>C10H19BF4N2</td>
<td>264.08</td>
<td>1-hexyl-3-methylimidazolium tetrafluoroborate;</td>
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<tr>
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<td>244193620</td>
<td>C12H23BF4N2</td>
<td>282.13</td>
<td>1-methyl-3-octylimidazolium tetrafluoroborate; 1-octyl-3-methylimidazolium tetrafluoroborate;</td>
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</table>

### Ions constituting the ionic liquid - 143314163

<table>
<thead>
<tr>
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<th>Formula</th>
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<th>Ionic Name</th>
<th>Structure</th>
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<td>BF4</td>
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<td>Borate(1-); tetrafluoro-; Fluoroborate; Tetrafluoroborate; Tetrafluoroborate (BF4-); Tetrafluoroborate anion; Tetrafluoroborate(1-);</td>
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<tr>
<td>56032034</td>
<td>C3H11N2</td>
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<td>1-Ethyl-3-methylimidazolium; 1-Methyl-3-ethylimidazolium; 1H-imidazolium, 1-ethyl-3-methyl-; 3-Ethyl-1-methylimidazolium;</td>
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</table>

### Available Properties for the Ionic Liquids - 143314163

<table>
<thead>
<tr>
<th>Select</th>
<th>Property Category</th>
<th>Description</th>
<th>References</th>
<th>Data Points</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Heat Capacity</td>
<td>Heat capacity at constant pressure, J/(K mol)</td>
<td>1</td>
<td>14</td>
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<tr>
<td></td>
<td>Phase Change Enthalpy</td>
<td>Enthalpy of transition or fusion, kJ/mol</td>
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<td>1</td>
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<tr>
<td></td>
<td>Thermal Properties</td>
<td>Thermal conductivity, W/(m·K)</td>
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<tr>
<td></td>
<td>Transport Properties</td>
<td>Viscosity, Pa·s</td>
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<tr>
<td></td>
<td>Temperature</td>
<td>Normal freezing point, K</td>
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<td>1</td>
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<tr>
<td></td>
<td>Volumetric Properties</td>
<td>Specific density, kg/m³</td>
<td>2</td>
<td>8</td>
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</tbody>
</table>
Data Summary

Property: Heat capacity at constant pressure, J/(K mol)
Compound: Name - 1-ethyl-3-methylimidazolium tetrafluoroborate; 1H imidazolium, 1-ethyl-3-methyl-, tetrafluoroborate(1-); [EMMI][BF4];
CASRN: 143314163  Formula - C6H11BF4N2

Total References: 1
Total Data Points: 14

References and Data Sets

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<th>Authors</th>
<th>Data Set</th>
<th>Data Type</th>
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<th>Variable2</th>
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<th>Phase2</th>
<th>Phase3</th>
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<tbody>
<tr>
<td>2005</td>
<td>Van Valkenburg, M. E.; Vaughn, R. L.; Williams, M.; Wilkes, J. S.</td>
<td>1</td>
<td>One Variable</td>
<td>Temperature, K</td>
<td>Liquid</td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

Purity and Measurement

Source: Synthesized by the author
Initial Purity: Not stated
Purification: Not stated
Final Purity: 99 mol %, .065 water mass %.113 halide impurity mass %
Purity Analysis: Spectroscopy, I f Acid-base titration
Measurement Purpose: Direct observation
Measurement Method: Small sample (50 mg) DSC

Selected Data Set (Property/Uncertainty - Heat capacity at constant pressure, J/(K mol))

<table>
<thead>
<tr>
<th>Year Pub</th>
<th>Data Set</th>
<th>Temperature, K</th>
<th>Property Value</th>
<th>Uncertainty</th>
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Title: Thermochemistry of ionic liquid heat-transfer fluids

Keywords: Ionic liquid; Heat capacity; Heat transfer; Thermal conductivity; Thermal stability

Abstract: Large-scale solar energy collectors intended for electric power generation require a heat-transfer fluid with a set of properties not fully met by currently available commercial materials. Ionic liquids have thermophysical and chemical properties that may be suitable for heat transfer and short heat term storage in power plants using parabolic trough solar collectors. Ionic liquids are salts that are liquid at or near room temperature. Thermal properties important for heat transfer applications are melting point, boiling point, liquidus range, heat capacity, heat of fusion, vapor pressure, and thermal conductivity. Other properties needed to evaluate the usefulness of ionic liquids are density, viscosity and chemical compatibility with certain metals. Three ionic liquids were chosen for study based on their range of solvent properties. The solvent properties correlate with solubility of water in the ionic liquids. The thermal and chemical properties listed above were measured or compiled from the literature. Contamination of the ionic liquids by impurities such as water, halides, and metal ions often affect physical properties. The ionic liquids were analyzed for those impurities, and the impact of the contamination was evaluated by standard addition. The conclusion is that the ionic liquids have some very favorable thermal properties compared to targets established by the Department of Energy for solar collector applications.
Anticipated Functionality from ILThermo

- Provide users worldwide with free internet access to literature information on experimental investigations on ionic liquids
- Assist researchers in their literature search, data evaluation, systematic studies on the direction of future investigations
- Allow chemical engineers access to complete and up-to-date physicochemical property data of ionic liquids