

Internet Connection

IUPAC Solubility Data on the Internet

A database containing solubilities originally published in the International Union for Pure and Applied Chemistry-National Institute of Standards and Technology (NIST) Solubility Data Series is now available at no cost online at <http://srdata.nist.gov/solubility>. This database, which is of significant value to analytical chemists, engineers, health scientists, and environmentalists, is derived from 11 volumes of the series and is concerned primarily with liquid-liquid systems. A limited number of multi-component (organic-water-salt) systems are also included.

Typical solvents and solutes include water, seawater, heavy water, inorganic compounds, and a variety of organic compounds such as hydrocarbons, halogenated hydrocarbons, alcohols, acids, esters, and nitrogen compounds. For many systems, sufficient data were available to allow critical evaluation.

About NIST and the Solubility Data Series

IUPAC's *Solubility Data Series* (SDS), begun in the mid-1970s, is an exhaustive compilation and critical evaluation of all the world's published results of experimental determinations of solubility. Since 1979, over 70 SDS volumes have been published, including evaluated data on the solubility of gases in liquids, liquids in liquids, and solids in liquids. These volumes represent one of the largest collections of chemical property data ever produced and are the result of the work of scientists throughout the world.

With the explosion of Web-based chemical information resources, IUPAC and NIST began discussions about how best to make the contents of the SDS available online and in 1999 concluded an agreement to achieve this. Over 70 printed volumes have been printed, many of which are not available in computerized format. This first subset to be made available online deals with the solubility of liquids in liquids and covers these 11 volumes:

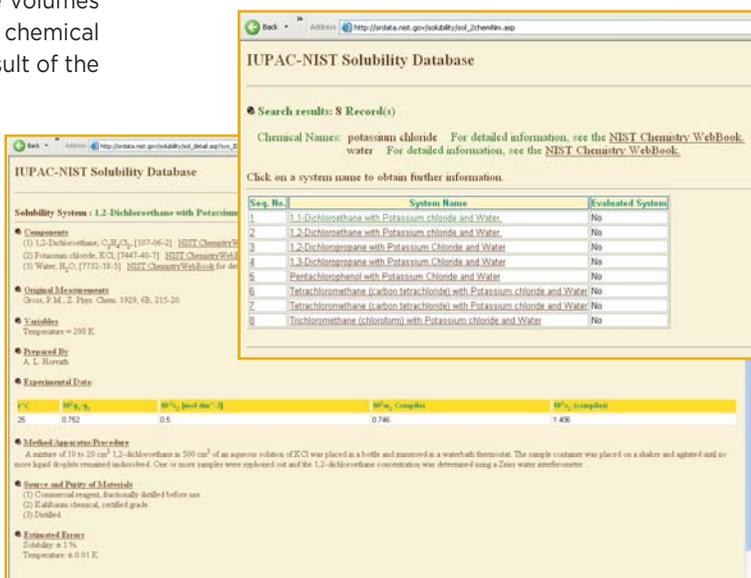
- SDS 20 "Halogenated Benzenes, Toluenes and Phenols with Water" (1985)

- SDS 37-38 "Hydrocarbons in Water and Seawater, Parts I-II" (1989)
- SDS 58-59 "Polycyclic Aromatic Hydrocarbons: Binary Non-aqueous Systems, Parts I-II" (1995)
- SDS 60 "Halogenated Methanes with Water" (1995)
- SDS 67 "Halogenated Ethanes and Ethenes with Water" (1999)
- SDS 68 "Halogenated Aliphatic Compounds C3-C14 with Water" (1999)
- SDS 69 "Ternary Alcohol-Hydrocarbon-Water Systems" (1999)
- SDS 71 "Binary Nitromethane Systems" (2000)
- SDS 77 "C2 + Nitroalkanes with Water or Organic Solvents: Binary and Multicomponent Systems" (2002)

Scope

The IUPAC-NIST Web site allows users to examine over 3600 multi-component systems containing over 1000 chemical substances. Many of the systems (over 338) have been critically evaluated. For these, the Web site presents reported numbers and best value data in tables, along with data correlation equations and graphical summaries. All of the critical evaluations include pertinent references taken from the compilation sheets. The database has over 800 references for the critical evaluations that can be searched for on the site. Chemical component searches are also supported, as well as system searches.

 <http://srdata.nist.gov/solubility/>



The screenshot displays the IUPAC-NIST Solubility Database search results for 'potassium chloride'. The search results table lists 8 records, with columns for 'Seq. No.', 'System Name', and 'Evaluated System'. The table shows various systems involving dichloroethane, dichloropropane, pentachlorophenol, tetrachloromethane, and trichloromethane with potassium chloride and water. The 'Evaluated System' column indicates 'No' for all listed systems.

Seq. No.	System Name	Evaluated System
1	1,1-Dichloroethane with Potassium chloride and Water	No
2	1,2-Dichloroethane with Potassium chloride and Water	No
3	1,3-Dichloropropane with Potassium Chloride and Water	No
4	1,3-Dichloropropane with Potassium Chloride and Water	No
5	Pentachlorophenol with Potassium Chloride and Water	No
6	Tetrachloromethane (carbon tetrachloride) with Potassium chloride and Water	No
7	Tetrachloromethane (carbon tetrachloride) with Potassium chloride and Water	No
8	Trichloromethane (chloroform) with Potassium chloride and Water	No