



Checking for the Availability of
Thermophysical Data

The Dortmund Data Bank

The Dortmund Data Bank (DDB) is a factual data bank for thermodynamic and thermophysical data compiled from primary sources like scientific publications, theses, company reports, deposited documents, and private communications. Only experimental data from the original publications are stored and all sources are available at DDBST GmbH.

Besides the easily accessible thermophysical properties from scientific literature (J. Chem. Eng. Data, J. Chem. Thermodyn., Fluid Phase Equilib., Thermochim. Acta, and Int. J. Thermophys.) DDB contains a great part of data not available via the open literature (systematic measurements for the development of predictive tools, private communications, confidential data from industry, BSc., MSc and PhD theses, ... from all over the world). These data will not be provided by online-services and are not made available to competitors of DDBST GmbH. The DDB offers vast amounts of information for a wide variety of applications in chemical engineering, environmental protection, and plant safety. It is especially valuable for the design of separation processes, e.g. distillation, extraction, absorption, crystallization, evaporation, ...

Besides covering the most common components the DDB contains data for e. g. ionic liquids, biofuel components, amines used in gas treating, polymers, electrolytes, and more.

Distribution Channels

The DDB is distributed as an in-house data bank together with a software package (DDBSP) for data retrieval, visualization, regression and export to other applications like spreadsheets or chemical process simulators. In addition, this software package includes many state-of-the-art property estimation models for pure component and mixture properties like UNIFAC, mod. UNIFAC, PSRK, VTPR, COSMO-RS(OI), COSMO-SAC as well as process synthesis tools and further utilities.

As a second distribution channel, the Dortmund Data Bank is used within our consulting services, either in form of simple data deliveries but more often in combination with advanced services like data regression (e. g. for g^E models like Wilson, NRTL and UNIQUAC or pure component vapor pressure equations like simple or extended Antoine, Wagner, heat capacity polynomial parameters, parameters for a variety of DIPPR and PPDS equations). Data are also bundled with specific available or custom-tailored software tools. In many cases, data are delivered together with property estimation results. In addition, missing data can be measured at our partner organization LTP GmbH.

Major parts of the Dortmund Data Bank except e.g. data bases for polymer data and adsorbent/adsorptive equilibria as well as many data supplied by the Gas Processors Association), are also included in DETHERM (i-systems.dechema.de).

The Online DDB Search

Online DDB Search has been developed to enable a world-wide access to the contents of the Dortmund Data Bank. The site allows checking for the availability of thermophysical data free of charge and in addition it offers qualified consulting beyond just data delivery upon request.

The screenshot shows the 'DDB Component Search' interface. At the top, there is a navigation menu with options like Home, Contact, About Us, News, DEHEMA Courses, Payments, DDB Search, Downloads, and Educational Version. Below the menu, there are search filters for Company, Products, Support, UNIFAC, GVT Courses, Meetings, Estimation, Info Material, and Printed Data Collections. The main search area has a search bar with 'methanol' entered and a 'Search' button. Below the search bar, there are fields for Name, CAS-RN, and Formula, each with a search button. The search results show 116 components found, with a table listing components like Methanol, Methanolamine, 2-Furanmethanol, Oxiranemethanol, m-Tolylmethanol, and p-Tolylmethanol. Below the table, there are 'Add to System' and 'Cancel' buttons. A 'Component' section shows details for component 161 Toluene, including its CAS-RN (108-88-3) and formula (C7H8), with a 'Delete' button. At the bottom, there is a version notice: 'Dortmund Data Bank Version: April 2009'.

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DDB Online Search is explicitly not a web shop and it is not possible to buy data through this service directly. DDB Online Search is designed as an information source only and request will always be answered by one of DDBST's employees.

Supported Data Banks

Online DDB Search covers the complete list of data types stored in the Dortmund Data Bank including phase equilibrium data (VLE, LLE, SLE, azeotropic data), gas and salt solubilities, activity coefficients at infinite dilution, octanol-water partition coefficients, volumes, densities, critical data of mixtures, and a large variety of data for salts, polymers, adsorbents and organic pure components. The DDB currently contains more than 178,000 pure component data sets with 1,209,000 data tuples. For mixtures more than 356,000 data sets with 2,538,000 data tuples are available (April 2009).

Typical Outputs

A typical output includes details about the data types, the temperature and pressure ranges, and the number of sets and points (where available).

This first example below shows all available data for the binary mixture of Ethanol and Methanol.

The second example shows all data for the pure component 1,3-dichloro-2-butene where only a few data are available.

Terms and Conditions of Use

Prices

DDBST GmbH provides Online DDB Search free of charge. Please take a look at the price lists for data sets, complete or partial data banks and software for further information.

Copyright

Online DDB Search results can be distributed freely and no copyright is reserved for the search results as long as they are distributed together with a link or reference to the DDB or Online DDB Search.

System/Mixture

DDB#	Name	CAS-RN	Formula
11	Ethanol	64-17-5	C ₂ H ₆ O
110	Methanol	67-56-1	CH ₄ O

Mixture Data

Databank	Sets	Points	Temperature [K]	Pressure [kPa]	
Vapor-Liquid Equilibria	VLE	57	805	295-409	500-5840
Heats of Mixing	HE	5	33	298-323	n. a.
Activity Coefficients at Infinite Dilution	ACT	8	8	298-424	n. a.
Excess Heat Capacities	CPE	3	21	298-441	101 (const.)
Azeotropic Data	AZD	45	45	273-433	40-1013
Solid-Liquid Equilibria	SLE	1	7	144-175	n. a.
Densities/Volumes/Excess Volumes	VE	25	285	283-338	101 (const.)
Total		144	1204		

(0.99 seconds)

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System/Mixture

DDB#	Name	CAS-RN	Formula
365	1,3-Dichloro-2-butene	926-57-8	C ₄ H ₆ Cl ₂

Pure Component Data

Property	Number of Points	Number of Sets	Temperature Range	States	Number of Sets
Vapor Pressure	23	5	T=307-401 K	Vapor-Liquid	5
Liquid Density	4	4	T=293-293 K	Liquid	4

(0.47 seconds)

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