

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 Ph.D. 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 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 organisation LTP GmbH.

Major parts of the Dortmund Data Bank except e.g. adsorbent/adsorptive equilibria as well as many data supplied by

the Gas Processors Association (GPA) 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 'Online DDB Search' interface. At the top, there is a header with the DDB logo and 'DDBST GmbH'. Below this, the page title is 'Online DDB Search' and 'Dortmund Data Bank'. There is a search form with the following fields: 'DDB No.', 'Name', 'CAS-RN', 'Formula', and 'SMILES'. Each field has a corresponding 'Search' button. Below the search form, there are instructions: 'Enter a DDB number, a name or part of name, a CAS registry no. or an empirical formula (case-sensitive preferred) to search for components', 'Search for multiple DDB numbers (separated by space) is possible', and '* "Name" accepts multiple search strings (but searches only a limited number of names per component)'. At the bottom, there is a footer with 'Dortmund Data Bank Version: December 2018' and '© Dortmund Data Bank by DDBST GmbH'.

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

The online DDB search covers the complete list of data banks of the Dortmund Data Bank. Included are the data banks for

- Pure component properties
 - P-v-T related data (vapor pressures, critical data, densities, virial coefficients, and more)
 - Transport properties (viscosities, thermal conductivities, ...)
 - Enthalpies (phase change, formation, ...)
 - Heat capacities
 - Surface tensions
 - and more

- Mixture properties
 - Vapor-liquid equilibria
 - Liquid-liquid equilibria (miscibility gaps)
 - Solid-liquid equilibria (solubilities)
 - Activity coefficient at infinite dilution
 - Gas solubilities
 - Azeotropic and zeotropic data
 - Heats of mixing
 - Densities, volumes and excess volumes
 - Excess heats of mixing
 - Critical data of mixture
 - Salt solubilities
 - Vapor-liquid equilibria for electrolyte containing mixtures
 - Octanol-water partition coefficients
 - Adsorbent/adsorptive equilibria
 - Polymer related information (covering phase equilibria data and more)
 - Dynamic and kinematic viscosities
 - Thermal conductivities
 - Speeds of sound
 - Surface tensions
 - Dielectric constants

The screenshot shows the 'Online DDB Search' interface. At the top, it says 'Dortmund Data Bank' and 'Contact DDBST +49 441 361819 0'. Below that, a 'Query' section shows 'Selected System/Mixture' with 'Ethanol' (CAS-63) and 'Methanol' (CAS-67). A table lists various data sets with columns for 'Database', 'Name', 'CAS-63', 'Formula', and 'Overview'. Below this is a 'Mixture Data' table with columns for 'Database', 'Sets', 'Points', 'Temperature Range', and 'Pressure Range'. A pie chart titled 'Properties Data Point Distribution' shows the following categories: (A)zeotropic Data (20.2%), Critical Data (24.7%), Diffusion Coefficients (12.7%), Heats of Mixing (10.7%), Mixture Phase Points (8.1%), Mixture P-T Data (10.7%), Mixture Surface Tension (10.7%), Mixture Thermal Conductivities (10.7%), Mixture Viscosities (10.7%), Solid-Liquid Equilibria (10.7%), and Vapor-Liquid Equilibria (10.7%).

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.

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 Ethyl tert-butyl ether where only a few data are available.

The screenshot shows the 'Online DDB Search' interface for a 'Selected Component' query. The component is 'Ethyl tert-butyl ether (ETBE)' with CAS-63 and formula C₈H₁₈O. A table lists various data sets with columns for 'Database', 'Name', 'CAS-63', 'Formula', and 'Overview'. Below this is a 'Pure Component Data' table with columns for 'Property', 'Points', 'Sets', 'Temperature Range', 'States', and 'Sets'. The table lists properties such as Critical Data, Density, Gibbs Energy of Formation, Heat of Vaporization, Melting Point, Molar Heat Capacity (Cp), Molar Saturation Heat Capacity, Speed of Sound, Std. Heat of Formation, Surface Tension, Vapor Pressure, Viscosity (Dynamic), and COSMO-RS or Profile.

Changes and errors are possible regarding all information.