DDBST
DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

DDBST - Dortmund Data Bank Software & Separation Technology GmbH
Marie-Curie-Str. 10 | D-26129 Oldenburg | Germany

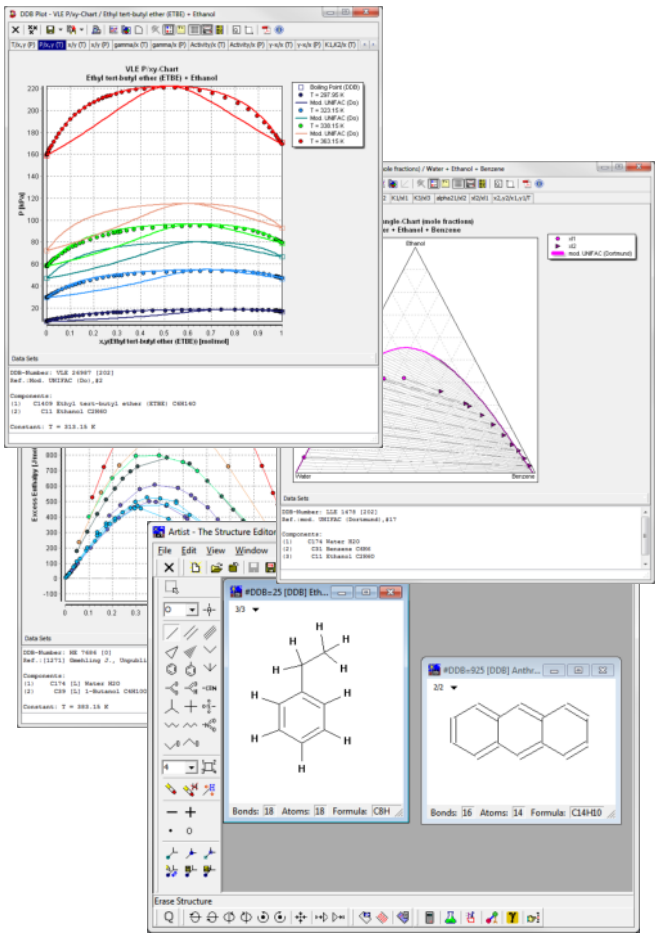
DDBSP 2017 – Educational Version

Teaching Physical Properties for Process Design and Simulation Using DDB and DDBSP

DDBSP – Educational Version is designed to be used for lectures and exercises and to give teachers and students nearly all the possibilities of the full Dortmund Data Bank (DDB) and the integrated software package (DDBSP). To achieve this for a small fraction of the price of the commercial version, some of the very complex and advanced features were left out and the experimental data banks are limited to 30 common components and their mixtures.

Nevertheless, this makes more than 79,500 real world data sets from the open literature and private communications available for examination, regression and graphical representation.
Using a large number of group contribution methods (like Joback, Ambrose, Benson, UNIFAC) or COSMO-RS (Ol) for pure and mixture properties (like VLE or LLE), data can easily be estimated from molecular structure. Just draw the molecule using our convenient structure editor ARTIST and click the property you need.

The package comes with extended documentation and course material (PowerPoint© slides).



Use this product to

- incorporate modern methods and data into teaching
- have your students examine real world experimental data
- let them get acquainted to experimental scattering and reliability of data
- get hands on experience with a large variety of estimation methods
- teach them to use the most sophisticated tool for physical property estimation, which is also used by many companies worldwide
- let them explore thermodynamic relationships between different types of data (e. g. pure component vapor pressures and enthalpy of vaporization)
- let them explore the performance of thermodynamic models for the simultaneous description of different types of data (VLE, h^E, ...)
- Search, regress, estimate, visualize, ... physical property data to be used in design projects

Major Data Types Volume (30 Components)

Abbrev.	Description	Datasets	Data points
VLE	Vapor - liquid equilibria	4,600	74,700
HPV	Vapor - liquid equilibria (normal boiling point of a component below 0°C)	3,600	30,400
ELE	Vapor - liquid equilibria for systems containing electrolytes	940	10,400
LLE	Liquid - liquid equilibria	2,700	19,700
ACT	Activity coefficients at infinite dilution (binary systems)	3,400	3,400
ACM	Activity coefficients at infinite dilution	170	1,100
GLE	Gas solubilities	1,700	7,800
EGLE	Gas solubilities (electrolyte containing systems)	400	2,400
SLE	Solid - liquid equilibria	1000	9,700
ESLE	Salt solubilities	1,300	6,000
AZD	Azeotropic / zeotropic information	5,470	5,470
...	...		

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Software & Separation Technology GmbH
Marie-Curie-Str. 10 | D-26129 Oldenburg | Germany
+49-441-361819-0
+49-441-361819-10
info@ddbst.de | www.ddbst.de

Oldenburgische Landesbank AG
Account No.: 142 6 164 800 | Bank Code: 280 200 50
SWIFT-BIC: OLBO DE H2 | IBAN: DE46 280 200 50 142 6 164 800
HRB Oldenburg 2521 | VAT Reg.No.: DE117 483996

Managing Directors:
Prof. Dr. Jürgen Gmehling,
Dr. Andreas Grybat, Dr. Sven Horstmann,
Dr. Christian Ihmels, Dr. Bastian Schmid

Major Features

- Ideal software package for teaching thermodynamics
- Contains a very large amount (approx. 79,500 data sets) of experimental pure component and mixture data from thousands of original references stored in the DDB
- The data bank is nearly complete for the components and mixtures included
- Simple to use Windows software for data retrieval, plotting, regression and estimation
- Basic data from the famous DDB (Antoine constants, critical data, acentric factor, density, UNIQUAC r and q values, CAS-RN) as well as several hundred molecular structures already included (53,000 for professional edition) as well as COSMO-RS sigma profiles for 27 components
- Calculation of VLE, h^E, azeotropic compositions, ... using correlative (Wilson, NRTL, UNIQUAC, ...) or predictive (UNIFAC, mod. UNIFAC, ASOG, PSRK, VTPR) methods
- Fast automatic pure component property estimation using 20 well known group contribution methods
- Automatic fragmentation of molecules into structural groups for a large number of group contribution methods including UNIFAC, mod. UNIFAC (Do) and ASOG
- Utilizes a user-friendly Windows graphical user interface
- Exports data to Microsoft Excel™

Available Data for the 30 Components

	References	Data Sets	Data Points
Vapor Pressure	4,100	7,100	34,700
Critical Data	380	680	680
Viscosity	2,600	6,600	36,200
Density	6,400	14,900	108,400
Melting Point	1,070	1,600	2,470
Heat Capacity	700	2,500	25,700
Enthalpy of Vaporization	220	470	1,760
Enthalpy of Fusion	150	220	240
Enthalpy of Sublimation	30	40	90
Thermal Conductivity	560	2,600	24,000
Surface Tension	560	1200	4,700
Entropy (various)	110	180	590
Enthalpy of Combustion	40	100	100
Enthalpy of Formation	60	120	300
Speed of Sound	1,300	3,000	18,400
G-Function	60	90	1,570
...			
Total	**14,300**	**41,800**	**265,600**

Components Included

Acetone, Ethanol, Ethyl Acetate, Benzene, Trichloromethane, Cyclohexane, n-Hexane, Methanol, Water, Carbon Dioxide, Methane, Sodium Chloride, 1-Butanol, NMP, iso-Propanol, Acetonitrile, Nitrogen, Potassium Chloride, Naphthalene, Sulfolane, Hexen-1, Hexadecane, p-Xylene, m-Xylene, Diethyl ether, Acetic Acid, Glycol, Butadiene, Butyl Acetate, Tetrahydrofuran

Licenses

Basic Educational Version – Features

Pure component and mixture **data** for 30 common components.
Includes data **retrieval** and **graphical representation** for all data banks.
Data Bank Add-On for Fitting and Plotting: Extended parameter **fitting**, **prediction** and **graphical representation** for VLE, h^E, LLE and azeotropic data. Includes **g^E models**, **equations of state** and **electrolyte** models.
Mixture Data Bank Add-On - Prediction Methods: Prediction of mixture data using **UNIFAC**, **mod. UNIFAC (Do)**, **ASOG**, **PSRK**. Extended graphical representations for multicomponent mixtures.
ARTIST (Basic Version): Pure component property **estimation from chemical structure** for 20 group contribution methods (like Joback and Benson), graphical editor for molecular structures, **structure data base** (approx. 300 structures).

One-year license for a single workstation	**300 €**
Unlimited license for a single workstation	**999 €**
For a 10 concurrent user classroom license, add	
One-year license	**64 €**
Unlimited license	**256 €**
For a 20 concurrent user classroom license, add	
One-year license	**98 €**
Unlimited license	**390 €**

Professional Educational Version – Features

Basic Educational Version plus pure component data files and molecular structures for about 53,000 components plus data input editors for experimental data.

One-year license for a single workstation	**760 €**
Unlimited license for a single workstation	**3040 €**
For a 10 concurrent user classroom license, add	
One-year license	**68 €**
Unlimited license	**272 €**
For a 20 concurrent user classroom license, add	
One-year license	**106 €**
Unlimited license	**420 €**

Changes and errors possible regarding all information and prices.

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