

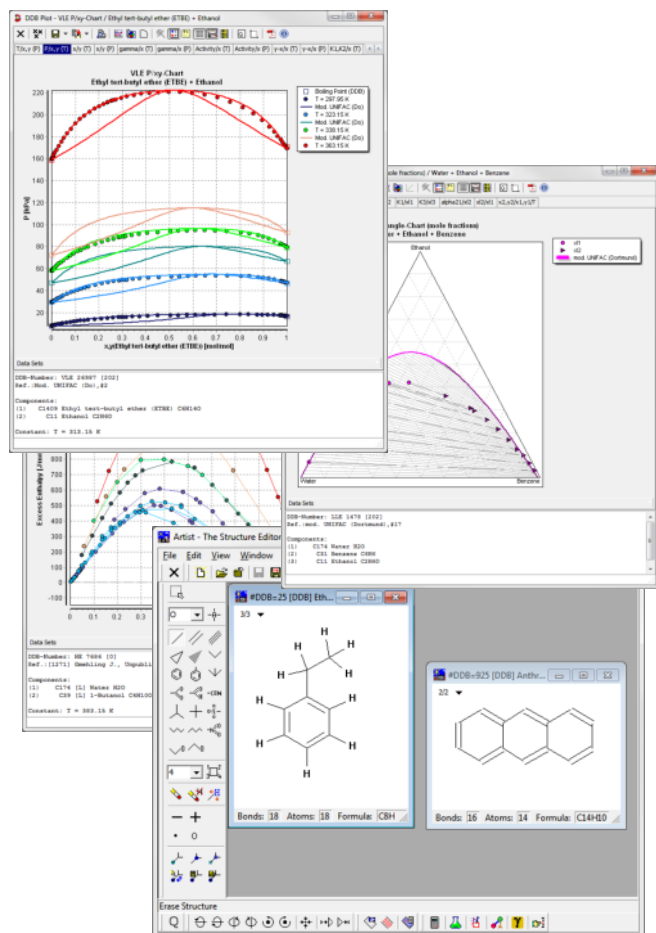


DDBSP – Educational Version is designed to be used for lectures and exercises and to give teachers and students nearly all the possibilities of the full Dortmund Data Bank (DDB) and the integrated software package (DDBSP). To achieve this for a small fraction of the price of the commercial version, some 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 81,300 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 (OI) 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	4,700	75,450
HPV	Vapor - liquid equilibria (normal boiling point of a component below 0°C)	3,800	31,650
ELE	Vapor - liquid equilibria for systems containing electrolytes	960	10,600
LLE	Liquid - liquid equilibria	2,800	20,200
ACT	Activity coefficients at infinite dilution (binary systems)	3,400	3,400
ACM	Activity coefficients at infinite dilution	170	1,100
GLE	Gas solubilities	1,750	8,000
EGLE	Gas solubilities (electrolyte containing systems)	440	2,550
SLE	Solid - liquid equilibria	1030	10,000
ESLE	Salt solubilities	1,350	6,200
AZD	Azeotropic / zeotropic information	5,500	5,500
...

Major Features

- Ideal software package for teaching thermodynamics
- Contains a very large amount (approx. 81,300 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	4,250	7,400	35,800
Critical Data	380	680	680
Viscosity	2,800	6,800	37,300
Density	6,600	15,300	110,600
Melting Point	1,090	1,650	2,500
Heat Capacity	700	2,550	25,700
Enthalpy of Vaporization	230	480	1,780
Enthalpy of Fusion	160	240	260
Enthalpy of Sublimation	35	45	95
Thermal Conductivity	570	2,630	24,100
Surface Tension	590	1250	4,950
Entropy (various)	110	180	590
Speed of Sound	1,450	3,250	19,300
G-Function	60	90	1,570
...			
Total	14,830	42,600	269,800

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

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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. 750 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 56,900 components plus data input editors for experimental data.

One-year license for a single workstation	780 €
Unlimited license for a single workstation	3120 €

For a 10 concurrent user classroom license, add

One-year license	70 €
Unlimited license	280 €

For a 20 concurrent user classroom license, add

One-year license	109 €
Unlimited license	430 €

Changes and errors possible regarding all information and prices.