

**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 47000 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 COSMORR (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.

## Use this product to

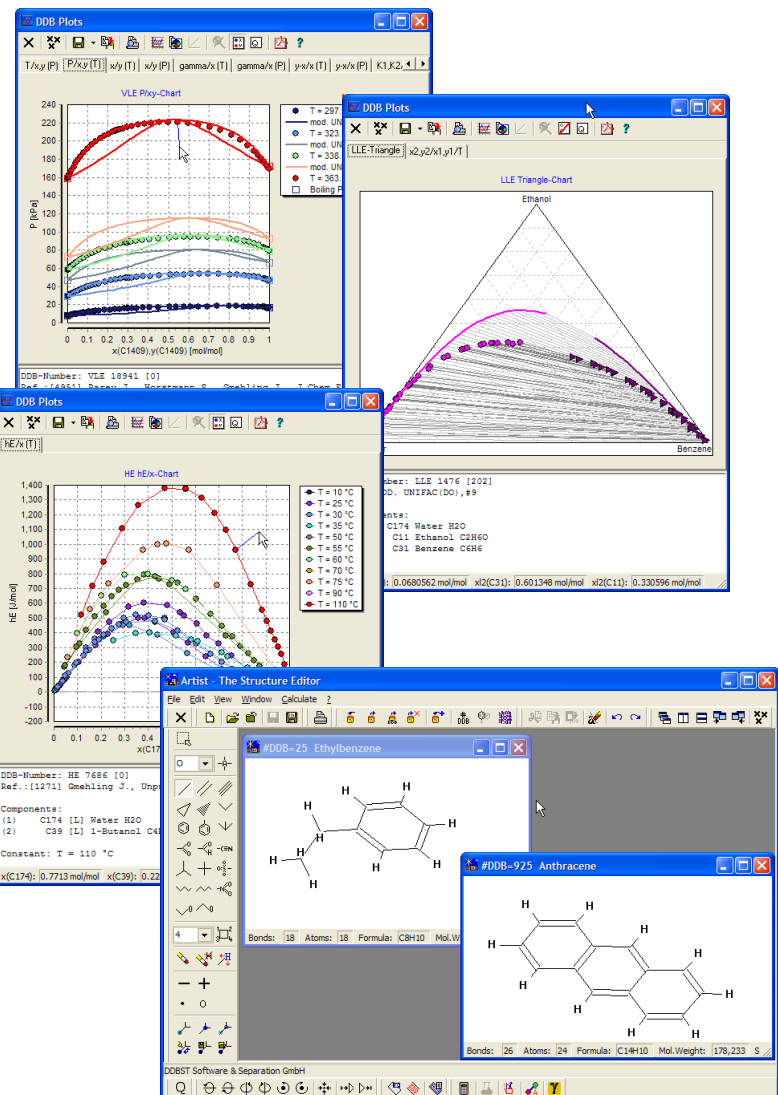
- incorporate modern methods and data into teaching
- have your students examine real world experimental data
- let them get acquainted to experimental scattering and reliability of data
- get hands on experience with a large variety of estimation methods
- teach them to use the most sophisticated tool 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,  $h^E$ ,  $\gamma^\infty$ , ...)

## Available Data for the 30 Components Included

Phase Equilibria	Description	Count	
Vapor-Liquid Equilibria	Normal Boiling Substances	3480	data sets
Vapor-Liquid Equilibria	Low Boiling Substances	2336	data sets
Vapor-Liquid Equilibria	Electrolyte Systems	426	data sets
Liquid-Liquid Equilibria		1909	data sets
Activity Coefficients	Infinite Dilution (Pure Solvents)	2881	data points
Activity Coefficients	Infinite Dilution (Solvent Mixtures)	129	data sets
Gas Solubilities		1264	data sets
Solid-Liquid Equilibria	Mainly Organic Compounds	494	data sets
Salt Solubilities	Mainly in Water	626	data sets
Azeotropic Data		4588	data points

## Excess/Other Properties

Excess Enthalpies	Heats of Mixing	2423	data sets
(Excess) Heat Capacities		286	data sets
(Excess) Volumes	Includes Volume Effect of Mixing	2932	data sets



## Major Features

- Ideal software package for teaching thermodynamics
- Contains a very large amount (approx. 47000 data sets) of experimental pure component and mixture data from thousands of original references as 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 (20000 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) 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 and ASOG
- Utilizes a user-friendly Windows graphical user interface
- Exports data to Microsoft Excel™

## System Requirements

Pentium III 500 MHz or higher PC, 120 MB of free hard disk space, 512 MB of RAM, Windows 2000/XP/Vista.

## Available Data for the 30 Components

Property	Data Sets	Data Points	Ref's
Critical Data	512	513	291
Vapor Pressure	4340	21913	2557
Enthalpy of Vaporization	426	1692	212
Melting Point	813	1070	501
Enthalpy of Fusion	121	127	90
Density	7381	68377	2581
2. Virial Coefficient	214	1035	130
Ideal Gas Heat Capacity	143	2043	99
Molar Heat Capacity	1769	14340	380
Entropy	134	222	95
Dielectric Constant	124	514	63
Viscosity	3541	19983	1200
Kinematic Viscosity	396	1297	101
Surface Tension	608	2654	246
Thermal Conductivity	2021	16516	408
...	...	...	...
Sum	23647	160789	

## 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, Diethylether, Acetic Acid, Glycol, Butadiene, Butyl Acetate, Tetrahydrofuran

## Licenses

### Basic Teaching Edition - Features

Pure component and mixture **data** for 30 common components.

Includes data **retrieval**, **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** and **equations of state** as well as **electrolyte models**.

Mixture Data Bank Add-On - Prediction Methods: Prediction of mixture data using **UNIFAC**, **mod. UNIFAC**, **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).

Yearly license for a single workstation	€ 250
Unlimited license for a single workstation	€ 999 <sup>1</sup>

### Professional Teaching Edition - Features

Basic Teaching Edition plus pure component data files and molecular structures for about 20000 components plus data input editors for experimental data.

Yearly license for a single workstation	€ 575
Unlimited license for a single workstation	€ 2290 <sup>1</sup>

## Classroom License

For a 10 concurrent user classroom license, add

Yearly license	€ 50
Unlimited license	€ 185 <sup>1</sup>

For a 20 concurrent user classroom license, add

Yearly license	€ 75
Unlimited license	€ 299 <sup>1</sup>

## Contact Information

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Visit our website to view additional information or download the documentation or the free DDB Data Directory.

<sup>1</sup> Updates are available once a year for 16<sup>2</sup>/<sub>3</sub> % of the price