DDBST
DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

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

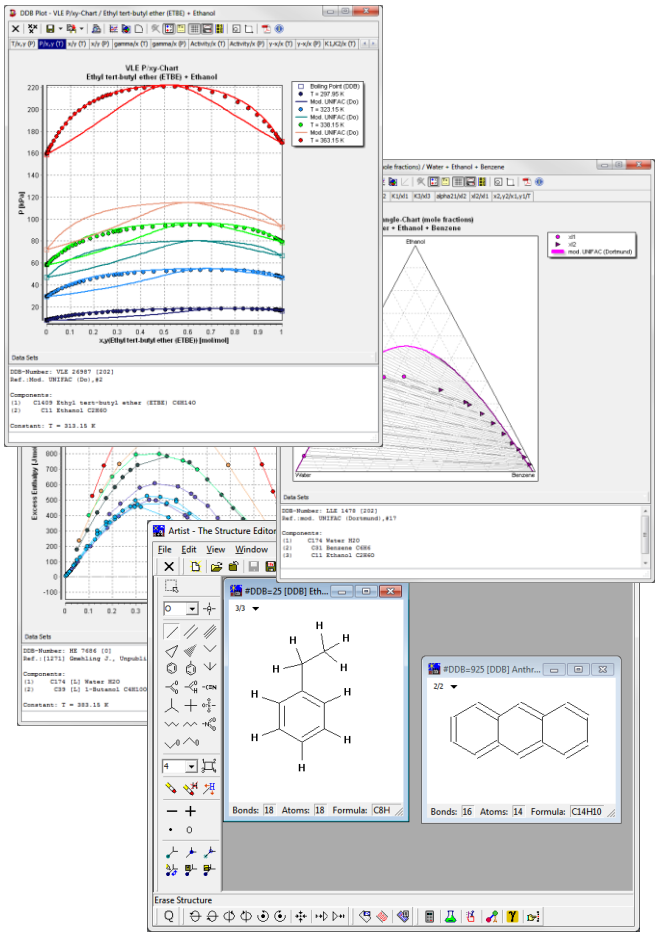
# DDBSP 2015 – Educational Version

## 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 57,000 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, hE, ...)
- Search, regress, estimate, visualize, ... physical property data to be used in design projects

**Major Data Types Volume (30 Components)**

| Abbrev. | Description | Datasets | Datapoints |
|---|---|---|---|
| VLE | Vapor - liquid equilibria | 4,398 | 71,403 |
| HPV | Vapor - liquid equilibria (normal boiling point of a component below 0°C) | 3,302 | 27,764 |
| ELE | Vapor - liquid equilibria for systems containing electrolytes | 735 | 7,895 |
| LLE | Liquid - liquid equilibria | 2,486 | 17,789 |
| ACT | Activity coefficients at infinite dilution (binary systems) | 3,323 | 3,323 |
| ACM | Activity coefficients at infinite dilution | 172 | 1,108 |
| GLE | Gas solubilities | 1,601 | 7,312 |
| EGLE | Gas solubilities (electrolyte containing systems) | 324 | 1,727 |
| SLE | Solid - liquid equilibria | 851 | 8,631 |
| ELSE | Salt solubilities | 1,124 | 5,269 |
| AZD | Azeotropic / zeotropic information | 5,249 | 5,249 |
| ... | ... | | |

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Jochen Menke, Dr. Bastian Schmid

## Major Features

- Ideal software package for teaching thermodynamics
- Contains a very large amount (approx. 57000 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 (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, 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 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 | 3,739 | 6,478 | 31,341 |
| Critical Data | 362 | 637 | 641 |
| Viscosity | 2,236 | 5,569 | 31,004 |
| Density | 5,467 | 13,202 | 100,274 |
| Melting Point | 962 | 1,466 | 2,087 |
| Heat Capacity | 651 | 2,387 | 24,157 |
| Enthalpy of Vaporization | 215 | 442 | 1,724 |
| Enthalpy of Fusion | 138 | 197 | 215 |
| Enthalpy of Sublimation | 33 | 41 | 93 |
| Thermal Conductivity | 534 | 2,535 | 23,437 |
| Surface Tension | 469 | 987 | 4,050 |
| Entropy (various) | 111 | 160 | 557 |
| Enthalpy of Combustion | 39 | 80 | 86 |
| Enthalpy of Formation | 66 | 103 | 165 |
| Speed of Sound | 1,014 | 2,489 | 15,396 |
| G-Function | 62 | 89 | 1,570 |
| ... | | | |
| **Total** | **16,098** | **36,862** | **236,797** |

## 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** 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**, **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 | **€ 300** |
| Unlimited license for a single workstation | € **999**[1] |

### *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 | **€ 720** |
| Unlimited license for a single workstation | **€ 2880**[2] |

### Classroom License

For a 10 concurrent user classroom license, add

| | |
|---|---|
| Yearly license | **€ 64** |
| Unlimited license | **€ 256**[2] |

For a 20 concurrent user classroom license, add

| | |
|---|---|
| Yearly license | **€ 98** |
| Unlimited license | **€ 390**[2] |

[1] Updates are available once a year for 15 % of the price in the preceding year

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