



DDBST

DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

DDBSP 2011 – Educational Version

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

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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 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).

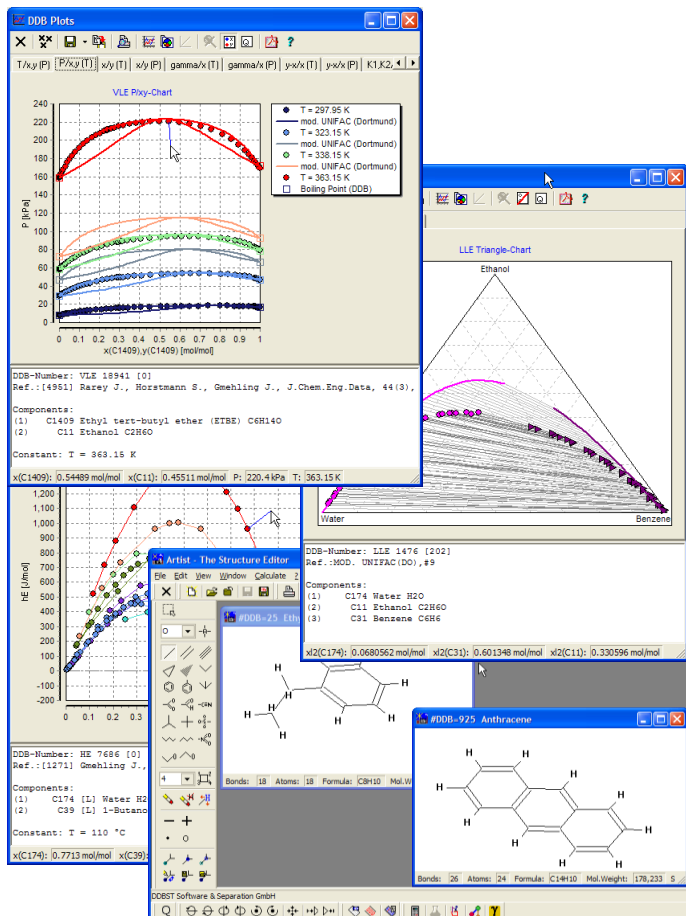
Use this product to

- 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 , γ^∞ , ...)
- Search, regress, estimate, visualize, ... physical property data to be used in design projects

Available Data for the 30 Components Included

Phase Equilibria	Description	Count	
Vapor-Liquid Equilibria	Normal Boiling Substances	3730	data sets
Vapor-Liquid Equilibria	Low Boiling Substances	2563	data sets
Vapor-Liquid Equilibria	Electrolyte Systems	525	data sets
Liquid-Liquid Equilibria		2046	data sets
Activity Coefficients	Infinite Dilution (Pure Solvents)	2943	data points
Activity Coefficients	Infinite Dilution (Solvent Mixtures)	129	data sets
Gas Solubilities		1346	data sets
Solid-Liquid Equilibria	Mainly Organic Compounds	589	data sets
Salt Solubilities	Mainly in Water	830	data sets
Azeotropic Data		4271	data points

Excess/Other Properties			
Excess Enthalpies	Heats of Mixing	2579	data sets
(Excess) Heat Capacities		336	data sets
(Excess) Volumes	Includes Volume Effect of Mixing	3566	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 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 free disk space, 512 MB RAM, Windows 2000/XP/Vista/7-32,64.

Available Data for the 30 Components

Property	Data Sets	Data Points	Ref's
Critical Data	535	536	311
Vapor Pressure	4750	23744	2772
Enthalpy of Vaporization	404	1664	198
Melting Point	903	1247	559
Enthalpy of Fusion	133	157	100
Density	8318	73888	2988
2. Virial Coefficient	230	1127	139
Ideal Gas Heat Capacity	146	2069	101
Molar Heat Capacity	1839	16360	410
Entropy	135	231	96
Dielectric Constant	393	2105	142
Dynamic Viscosity	3461	21413	1306
Kinematic Viscosity	402	1322	106
Surface Tension	660	2864	273
Thermal Conductivity	2048	17851	416
...
Sum	26073	177483	

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, 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 € 280

Unlimited license for a single workstation € 999¹

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 € 640

Unlimited license for a single workstation € 2560¹

Classroom License

For a 10 concurrent user classroom license, add

Yearly license € 56

Unlimited license € 224¹

For a 20 concurrent user classroom license, add

Yearly license € 83

Unlimited license € 332¹

Contact Information

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

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