DDB

DDBST
Dortmund Data Bank
Software & Separation
Technology

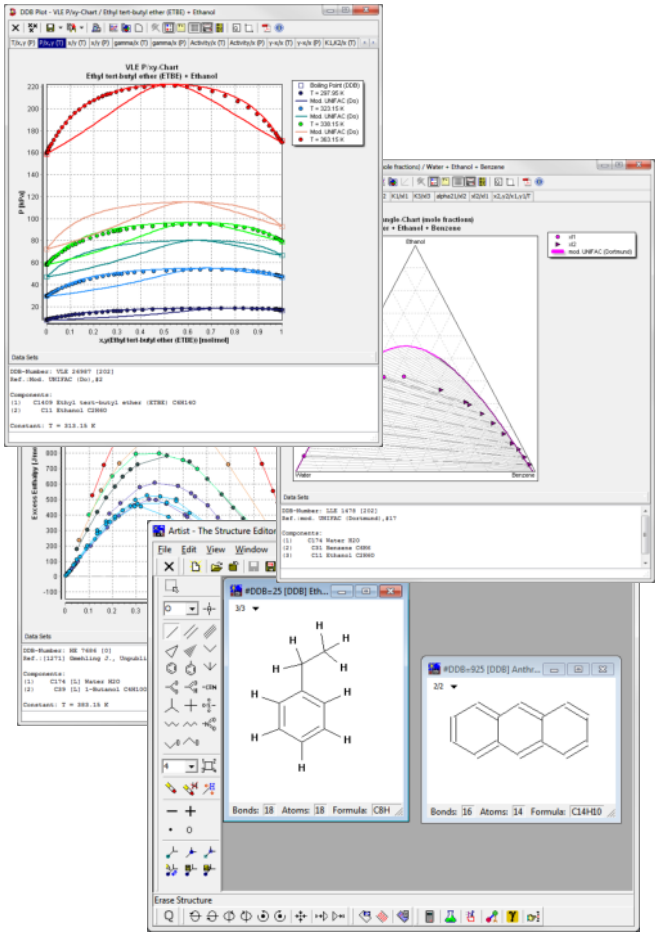
Educational Version 2021

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 82,700 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	4,800	77,400
HPV	Vapor - liquid equilibria (normal boiling point of a component below 0°C)	4,200	34,800
ELE	Vapor - liquid equilibria for systems containing electrolytes	1,000	12,000
LLE	Liquid - liquid equilibria	3,000	22,100
ACT	Activity coefficients at infinite dilution (binary systems)	3,500	3,500
ACM	Activity coefficients at infinite dilution	170	1,100
GLE	Gas solubilities	1,900	8,800
EGLE	Gas solubilities (electrolyte containing systems)	470	2,900
SLE	Solid - liquid equilibria	1,100	10,600
ESLE	Salt solubilities	1,400	6,500
AZD	Azeotropic / zeotropic information	5,600	5,600
...	...		

Major Features

- Ideal software package for teaching thermodynamics
- Contains a very large amount (approx. 82,700 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 (61,200 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, 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 and mod. UNIFAC (Do)
- 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	4,600	8,000	38,100
Critical Data	400	700	700
Viscosity	2,950	7,300	39,900
Density	7,400	16,800	119,000
Melting Point	1,100	1,700	2,600
Heat Capacity	700	2,700	27,700
Enthalpy of Vaporization	230	490	1,800
Enthalpy of Fusion	170	250	270
Enthalpy of Sublimation	35	45	130
Thermal Conductivity	600	2,700	26,300
Surface Tension	680	1,400	5,500
Entropy (various)	110	180	590
Speed of Sound	1,700	3,700	22,200
G-Function	60	90	1,570
...			
Total	**16,300**	**45,800**	**289,400**

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, Tetrahydro-furan

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)**, **PSRK**. Extended graphical representations for multicomponent mixtures.
ARTIST: 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. 72,500 structures).
Includes also data input editors for experimental data.

Licenses

- One-year license for a single workstation
- 10 concurrent user classroom license
- 20 concurrent user classroom license

Changes and errors possible regarding all information.