



# DDBST

Dortmund Data Bank  
Software & Separation  
Technology

DDBST –  
Dortmund Data Bank  
Software & Separation  
Technology GmbH

Marie-Curie-Str. 10  
26129 Oldenburg  
Germany

[www.ddbst.com](http://www.ddbst.com)

Phone +49 441 36 18 19 - 0  
Fax +49 441 36 18 19 - 10  
contact@ddbst.com

## Product Overview 2022

Dortmund Data Bank Access Packages	
<b>DDB Access Package</b>	This essential component of the <i>Dortmund Data Bank Access Package</i> provides data storage, data input editors, retrieval, graphical representation, import / export for all data banks. Available data bank modules are summarized on page two.
<b>+ Regression Pure</b>	The regression add-on for pure component properties allows extended parameter fitting, calculation and graphical representation for various correlations for different pure component properties including DIPPR, PPDS and simulator specific equations.
<b>+ Predictive Methods</b>	The predictive methods UNIFAC, mod. UNIFAC (Do), PSRK, VTPR, COSMO-SAC, COSMO-RS(OI) and calculations using NRTL, Wilson, UNIQUAC, EOS, Aspen Plus®, Pro/II™, Simulis® Thermodynamics and UniSim® Design (simulators are not part of the delivery) are provided to estimate mixture properties. $\sigma$ -profiles for 25 components, <i>GC2GE</i> and <i>Predict Mix</i> are included.
<b>Educational Version</b>	This special version based on the <i>DDB Access Package</i> is designed for academic use: It provides nearly all possibilities of the full Dortmund Data Bank and software tools for a moderate pricing. 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. It is only to be licensed by universities and can be expanded to include all available modules as full versions. Classroom licenses for a comprehensive introduction of chemistry and chemical engineering students to thermophysical properties, their correlation and estimation are available on request.

Dortmund Data Bank Advanced Packages	
<b>Regression Mix</b>	A powerful regression tool that provides simultaneous correlation of VLE, $h^E$ , $c_p^E$ , $\gamma^r$ , azeotropic data, LLE, and SLE of eutectic systems using $g^E$ -models (Wilson, NRTL, UNIQUAC, ...) including extended graphical representations.
<b>Regression Mix EOS</b>	A powerful regression tool that provides simultaneous correlation of VLE, $h^E$ , $c_p^E$ , $\gamma^r$ , azeotropic data, LLE, and SLE of eutectic systems using equations of state including extended graphical representations.
<b>Process Synthesis</b>	Apply process synthesis to new column designs with residual curves, constant property lines and calculation of azeotropic points in multi-component systems.
<b>Entrainer Selection</b>	Selection of selective solvents by data bank access or thermodynamic models.

Stand-Alone Software Tools	
<b>Predict Pure</b>	Pure Component property estimation software that also provides a molecular structure editor, data base (structures and basic data for 30 components), automatic group fragmentation, and property estimation from chemical structure (approx. 100 different methods) including method quality estimation for several important properties.
<b>+ Structures</b>	This add-on significantly enhances the <i>Predict Pure</i> property estimation methods by providing molecular structures for more than 80,500 compounds.
<b>Predict Mix</b>	Flash calculation and prediction of VLE, P/T curves, GLE, SCF, LLE, SLE, $\gamma$ , $\gamma^r$ , $h^E$ , $v^E$ and $c_p^E$ for mixtures up to 50 components. Available models: VTPR, PSRK, EOS, UNIFAC, mod. UNIFAC (Do), mod. UNIFAC (Ly), NIST mod. UNIFAC. Some properties cannot be calculated with all models. <i>Predict</i> is included in <i>Predictive Methods</i> .
<b>GC2GE</b>	Automatic generation of constant or temperature dependent $g^E$ -model parameters (Wilson, NRTL, UNIQUAC) from predictive methods (UNIFAC, mod. UNIFAC (Do), NIST-modified UNIFAC, COSMO-SAC, COSMO-RS (OI)). <i>GC2GE</i> is included in <i>Predictive Methods</i> .
<b>Flash Point Estimation</b>	Enables the estimation of flash points of flammable liquid mixtures using UNIFAC, mod. UNIFAC (Do), NIST-modified UNIFAC, Wilson, NRTL and UNIQUAC for systems with up to 50 components. Flash Points for 1,220 components are included.

System requirements: Official supported Microsoft Windows versions at release time.  
Changes and errors possible regarding all information and prices.

DDBST GmbH  
HRB Oldenburg 2521  
TAX ID: DE 117483996

Board of Executive Directors:  
Dr. Andreas Grybat, Dr. Sven Horstmann,  
Dr. Christian Ihmels, Dr. Bastian Schmid

Oldenburgische Landesbank AG  
Account: 142 61648 00  
Bank Code: 280 200 50  
SWIFT-BIC: OLBO DE H2  
IBAN: DE46 2802 0050 1426 1648 00

Dortmund Data Bank Modules, Mixture Data			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	43,000
Vapor-Liquid Equilibria	low boiling substances	HPV	48,800
Vapor-Liquid Equilibria	electrolyte systems	ELE	14,950
Liquid-Liquid Equilibria		LLE	39,850
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(125,000)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	2,050
Gas Solubilities	in non-electrolyte systems	GLE	30,540
Gas Solubilities	in electrolyte systems	EGLE	4,750
Critical Data of Mixtures	critical lines	CRI	4,250
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	86,750
Salt Solubilities	in electrolyte systems	ESLE	50,000
Azeotropic Data	in non-electrolyte systems	AZD	(60,550)
Partition Coefficients	octanol-water partition coefficients	KI	(15,200)
Adsorption Equilibria	vapor phase	AAE	5,900
Polymer Mixtures		POLYMER	23,250
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	24,750
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	7,650
Mixture Densities	includes also excess volumes	VE	88,200
Mixture Viscosities	includes also viscosity deviations	VIS	66,700
Thermal Conductivities (Mixtures)		MTCN	5,750
Surface Tensions (Mixtures)		MSFT	10,100
Flash Points of Flammable Liquid Mixtures		MFLP	1,100
Speeds of Sound (Mixtures)		MSOS	35,250
Dielectric constants (Mixtures)		MDEC	8,500
Gas Hydrates		GHD	6,150
Mixture PvT		MPVT	22,350
Mixture Electrical Conductivity		ECND	15,000
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	59,150

Dortmund Data Bank Modules, Pure Component Properties		Data Sets	Components
<b>PCP-VAP+</b>	Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	153,250	50,100
<b>PCP-VIS+</b>	Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	47,800	6,350
<b>PCP-HCP+</b>	Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	55,550	14,100
<b>PCP-PVT+</b>	Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	107,450	17,500
<b>PCP-ENTH</b>	Enthalpies of Combustion and Formation, several types of Entropies, Enthalpies, Energies	21,250	7,550
<b>PCP-SFT</b>	Surface Tensions	8,850	3,350
<b>PCP-Other</b>	Dielectric Constants, Diffusion Coefficients, Flash Points, Dipole Moments, Molar Polarization	10,100	2,150

Upon Request	
<b>Special Pre-Tailored Data Subsets</b>	Biodiesel, Ionic Liquids, Mercury, Carbon Dioxide, Pharmaceuticals, or subsets of the various mixture data banks e.g. for a list of selected compounds.
<b>Vapor Phase Adsorption Software</b>	For the correlation of adsorption on different adsorption agents with the help of different pure components (e.g. Freundlich, Langmuir, BET, Toth) adsorption models.
<b>Basic Pure Component Data Files</b>	Basic data for calculations (critical data, Antoine constants, melting points, heats of fusion, CAS numbers, group definitions (UNIFAC, mod. UNIFAC (Do), ...) where available.
<b>PCP Correlation Parameters</b>	Correlation parameters for pure component properties (e.g. Antoine-, Vogel- or DIPPR105 equation)
<b>BIP's</b>	DDBST offers the fitting of binary interaction parameters to experimental data (e.g. NRTL, EOS, ...).
<b><math>\sigma</math>-Profiles</b>	A library of 4,435 $\sigma$ -profiles is provided for use with COSMO-SAC and COSMO-RS(OI).
<b>Solvent selection</b>	The selection of suitable solvents for separation processes using experimental data and predictive methods is available upon request.
<b>Consulting</b>	DDBST offers consulting and can be engaged for special projects.