



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

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

Product Overview 2023

Dortmund Data Bank Access Packages	
DDB Access Package	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.
+ Regression Pure	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.
+ Predictive Methods	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. σ -profiles for 25 components, <i>GC2GE</i> and <i>Predict Mix</i> are included.
Educational Version	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	
Regression Mix	A powerful regression tool that provides simultaneous correlation of VLE, h^E , c_p^E , γ^r , azeotropic data, LLE, and SLE of eutectic systems using g^E -models (Wilson, NRTL, UNIQUAC, ...) including extended graphical representations.
Regression Mix EOS	A powerful regression tool that provides simultaneous correlation of VLE, h^E , c_p^E , γ^r , azeotropic data, LLE, and SLE of eutectic systems using equations of state including extended graphical representations.
Process Synthesis	Apply process synthesis to new column designs with residual curves, constant property lines and calculation of azeotropic points in multi-component systems.
Entrainer Selection	Selection of selective solvents by data bank access or thermodynamic models.

Stand-Alone Software Tools	
Predict Pure	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.
+ Structures	This add-on significantly enhances the <i>Predict Pure</i> property estimation methods by providing molecular structures for more than 86,800 compounds.
Predict Mix	Flash calculation and prediction of VLE, P/T curves, GLE, SCF, LLE, SLE, γ , γ^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> .
GC2GE	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> .
Flash Point Estimation	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	43,800
Vapor-Liquid Equilibria	low boiling substances	HPV	50,200
Vapor-Liquid Equilibria	electrolyte systems	ELE	15,100
Liquid-Liquid Equilibria		LLE	40,950
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(126,750)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	2,450
Gas Solubilities	in non-electrolyte systems	GLE	31,300
Gas Solubilities	in electrolyte systems	EGLE	4,900
Critical Data of Mixtures	critical lines	CRI	4,300
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	92,800
Salt Solubilities	in electrolyte systems	ESLE	52,000
Azeotropic Data	in non-electrolyte systems	AZD	(61,300)
Partition Coefficients	octanol-water partition coefficients	KI	(15,350)
Adsorption Equilibria	vapor phase	AAE	6,150
Polymer Mixtures		POLYMER	23,750
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	24,900
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	7,850
Mixture Densities	includes also excess volumes	VE	90,200
Mixture Viscosities	includes also viscosity deviations	VIS	71,050
Thermal Conductivities (Mixtures)		MTCN	6,000
Surface Tensions (Mixtures)		MSFT	10,800
Flash Points of Flammable Liquid Mixtures		MFLP	1,440
Speeds of Sound (Mixtures)		MSOS	38,600
Dielectric constants (Mixtures)		MDEC	8,650
Gas Hydrates		GHD	6,550
Mixture PvT		MPVT	23,100
Mixture Electrical Conductivity		ECND	16,850
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	66,800

Dortmund Data Bank Modules, Pure Component Properties		Data Sets	Components
PCP-VAP+	Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	163,100	54,600
PCP-VIS+	Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	48,900	6,600
PCP-HCP+	Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	59,900	15,250
PCP-PVT+	Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	110,350	18,200
PCP-ENTH	Enthalpies of Combustion and Formation, several types of Entropies, Enthalpies, Energies	22,450	8,100
PCP-SFT	Surface Tensions	9,100	3,450
PCP-Other	Dielectric Constants, Diffusion Coefficients, Flash Points, Dipole Moments, Molar Polarization	10,250	2,200

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

License types:

- 7-year license without maintenance:
One-off payment of the basic price.
- 7-year license including maintenance:
Constant yearly fee, no price increase: 26.5% of the basic price
- One-year license (only for companies):
Yearly fee: 25% of the current basic price.

3- or 5-year contracts are available on request.

License renewals / maintenance:

- After a period of 7 years including maintenance, license renewals are available for 12.5% of the basic price.
- In case of yearly license renewals an auto-continuation contract limits the yearly price increase to 2.5%. The auto-continuation contract can be terminated on a yearly basis latest 3 months before the renewal date.

Surcharge for License Extensions:

- 2 PCs or 1 concurrent user: + 50%
- 3 PCs or 2 concurrent users: + 80%
- Site license: + 150%
- General license: + 250%

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