



## Product Overview 2026

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, $h^E$ , $c_p^E$ , $\gamma^\infty$ , 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, $h^E$ , $c_p^E$ , $\gamma^\infty$ , 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 thermodynamic models.
<b>+ Data Bank add-on</b>	This add-on significantly enhances the applicability of the <i>Entrainer Selection</i> package. It contains the experimental literature data bank modules <i>ACT</i> , <i>AZD</i> , <i>GLE</i> , <i>HPV</i> and <i>LLE</i> in an <i>Entrainer Selection</i> readable format for a fractional price of the full-versions.

Stand-Alone Software Tools	
<b>Predict Pure</b>	Pure Component property estimation software that also provides a molecular structure editor, database (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 115,000 compounds.
<b>Predict Mix</b>	Flash calculation and prediction of VLE, P/T curves, GLE, SCF, LLE, SLE, $\gamma$ , $\gamma^\infty$ , $h^E$ , $v^E$ 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. Predict 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.

Dortmund Data Bank Modules, Mixture Data			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	46,400
Vapor-Liquid Equilibria	low boiling substances	HPV	54,950
Vapor-Liquid Equilibria	electrolyte systems	ELE	16,050
Liquid-Liquid Equilibria		LLE	43,950
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(129,100)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	3,000
Gas Solubilities	in non-electrolyte systems	GLE	33,900
Gas Solubilities	in electrolyte systems	EGLE	5,300
Critical Data of Mixtures	critical lines	CRI	4,500
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	107,000
Salt Solubilities	in electrolyte systems	ESLE	55,750
Azeotropic Data	in non-electrolyte systems	AZD	(62,750)
Partition Coefficients	octanol-water partition coefficients	KI	(15,850)
Adsorption Equilibria	vapor phase	AAE	7,000
Polymer Mixtures		POLYMER	25,450
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	26,050
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	8,800
Mixture Densities	includes also excess volumes	VE	95,350
Mixture Viscosities	includes also viscosity deviations	VIS	85,800
Thermal Conductivities (Mixtures)		MTCN	7,050
Surface Tensions (Mixtures)		MSFT	13,900
Flash Points of Flammable Liquid Mixtures		MFLP	2,100
Speeds of Sound (Mixtures)		MSOS	48,400
Dielectric constants (Mixtures)		MDEC	11,450
Gas Hydrates		GHD	7,600
Mixture PvT		MPVT	31,400
Mixture Electrical Conductivity		ECND	30,400
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	99,850

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	223,000	80,700
<b>PCP-VIS+</b>	Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	51,550	7,100
<b>PCP-HCP+</b>	Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	95,500	26,500
<b>PCP-PVT+</b>	Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	119,750	20,050
<b>PCP-ENTH</b>	Enthalpies of Combustion and Formation, several types of Entropies, Enthalpies, Energies	25,350	8,900
<b>PCP-SFT</b>	Surface Tensions	9,800	3,700
<b>PCP-Other</b>	Dielectric Constants, Diffusion Coefficients, Flash Points, Dipole Moments, Molar Polarization	11,250	2,400

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.

Changes and errors possible regarding all information.