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 2020

Dortmund Data Bank Access Packages	
Basic Version (1.1)	This essential component of the Dortmund Data Bank Software Package (DDBSP) provides data storage, data input editors, retrieval, graphical representation, import / export for all data banks. Available data bank modules are summarized on the following page.
+ Basic Pure Component Data Files (1.2)	Data are provided for approximately 70,400 normal components, 9,400 salts, 620 polymer families with basic data for calculations (critical data, Antoine constants, melting points, heats of fusion, CAS numbers, group definitions (UNIFAC, mod. UNIFAC (Do), …) where available.
+ Regression Pure (1.3) (Pure Component Properties)	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 (1.5) (Mixture Properties)	The predictive methods UNIFAC, mod. UNIFAC (Do), ASOG, PSRK, VTPR, COSMO-SAC, COSMO-RS(Ol) and calculations using Aspen Plus®, Pro/II™, Simulis® Thermodynamics and UniSim® Design (simulators are not part of the delivery) are provided to estimate data and binary parameters (incl. σ-profiles for 25 components and GC2GE (2.5)).
++ σ-Profiles (1.8) (COSMO-RS, COSMO-RS(Ol))	A library of 4,435 σ-profiles is provided for use with COSMO-SAC and COSMO-RS(Ol).

Dortmund Data Bank Advanced Packages	
RECPAR (1.6a)	A powerful regression tool that provides simultaneous correlation of VLE, h^E, c_P^E, γ^∞, azeotropic data, LLE, and SLE of eutectic systems using g^E - models (Wilson, NRTL, UNIQUAC, …) including extended graphical representations.
RECPAR EOS (1.6b)	A powerful regression tool that provides simultaneous correlation of VLE, h^E, c_P^E, γ^∞, azeotropic data, LLE, and SLE of eutectic systems using equations of state including extended graphical representations.
Process Synthesis (1.7)	Apply process synthesis to new column designs with residual curves, constant property lines and calculation of azeotropic points in multi-component systems.
Entrainer Selection (1.9)	Selection of selective solvents by data bank access or using thermodynamic models.

ARTIST Property Estimation Software	
Basic Version (2.1)	Pure Component property estimation software that also provides a graphical user interface for DDBSP including 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 (2.2)	This add-on significantly enhances the ARTIST property estimation methods by providing molecular structures for more than 67,700 compounds.

Stand-Alone Software Tools	
Predictive GCEOS (2.3)	Flash calculation and prediction of vapor-liquid equilibria, gas solubilities, phase envelopes, mixing enthalpies, excess volumes and SCF with VTPR and PSRK.
UNIFAC (2.4)	Enables the estimation of activity coefficients, h^E and c_P^E with UNIFAC, mod. UNIFAC (Do) and NIST-modified UNIFAC for systems with up to 50 components.
GC2GE (2.5)	Automatic generation of constant or temperature dependent g^E-model parameters (Wilson, NRTL, UNIQUAC) from predictive methods (UNIFAC, mod. UNIFAC (Do), NIST-modified UNIFAC, ASOG, COSMO-SAC, COSMO-RS (Ol)). GC2GE is included in 1.5.
Flash Point Estimation (2.6)	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.

Product Overview 2020

Dortmund Data Bank Modules, Mixture Data			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	41,450
Vapor-Liquid Equilibria	low boiling substances	HPV	46,150
Vapor-Liquid Equilibria	electrolyte systems	ELE	14,450
Liquid-Liquid Equilibria		LLE	36,900
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(115,350)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	2,000
Gas Solubilities	in non-electrolyte systems	GLE	27,950
Gas Solubilities	in electrolyte systems	EGLE	4,350
Critical Data of Mixtures	critical lines	CRI	3,500
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	74,000
Salt Solubilities	mainly in water	ESLE	46,150
Azeotropic Data	in non-electrolyte systems	AZD	(59,500)
Partition Coefficients	octanol-water partition coefficients	KI	(15,050)
Adsorption Equilibria	vapor phase	AAE	5,400
Polymer Mixtures		POLYMER	22,350
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	24,150
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	7,250
Mixture Densities	includes also excess volumes	VE	84,100
Mixture Viscosities	includes also viscosity deviations	VIS	59,500
Thermal Conductivities (Mixtures)		MTCN	5,350
Surface Tensions (Mixtures)		MSFT	8,850
Flash Points of Flammable Liquid Mixtures		MFLP	810
Speeds of Sound (Mixtures)		MSOS	30,700
Dielectric constants (Mixtures)		MDEC	8,050
Gas Hydrates		GHD	5,500
Mixture PvT		MPVT	19,600
Mixture Electrical Conductivity		ECND	13,000
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	51,350

Dortmund Data Bank Modules, Pure Component Properties		Data Sets	Components
PCP-VAP+	Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	136,100	43,500
PCP-VIS+	Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	46,000	5,950
PCP-HCP+	Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	49,100	12,350
PCP-PVT+	Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	101,150	15,950
PCP-ENTH	Enthalpies of Combustion and Formation, Several Types of Entropies, Enthalpies, Energies	19,700	6,750
PCP-SFT	Surface Tensions	8,550	3,250
PCP-Other	Dielectric Constants, Diffusion Coefficients, Flash Points, Dipole Moments, Molar Polarization	9,700	2,100

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.
Educational Versions (3.X)	DDBST provides universities extensive single PC and classroom packages with training material for comprehensive introduction of chemistry and chemical engineering students to thermophysical properties, their correlation and estimation.
Vapor Phase Adsorption Software (4.1)	For the correlation of adsorption on different adsorption agents with the help of different pure components (e.g. Freundlich, Langmuir, BET, Toth) adsorption models.
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, …).
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.

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