DDB

DDBST

Dortmund Data Bank
Software & Separation
Technology

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Product Overview 2021

Dortmund Data Bank Access Packages	
DDB Access Package	This essential component of the *Dortmund Data Bank Access Package* 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), ASOG, PSRK, VTPR, COSMO-SAC, COSMO-RS(Ol) 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, *GC2GE* and *Predict Mix* are included.

Dortmund Data Bank Advanced Packages	
RECPAR (Regression Mix)	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 (Regression Mix)	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	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	
Artist (Predict Pure)	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	This add-on significantly enhances the ARTIST property estimation methods by providing molecular structures for more than 72,500 compounds.
Predict Mix	Flash calculation and prediction of VLE, P/T curves, GLE, SCF, LLE, SLE, γ, γ^∞, 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 *Predictive Methods*.
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, ASOG, COSMO-SAC, COSMO-RS (Ol)). *GC2GE* is included in *Predictive Methods*.
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.

Dortmund Data Bank Modules, Mixture Data			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	42,400
Vapor-Liquid Equilibria	low boiling substances	HPV	47,450
Vapor-Liquid Equilibria	electrolyte systems	ELE	14,650
Liquid-Liquid Equilibria		LLE	38,250
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(121,450)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	2,050
Gas Solubilities	in non-electrolyte systems	GLE	28,750
Gas Solubilities	in electrolyte systems	EGLE	4,450
Critical Data of Mixtures	critical lines	CRI	3,550
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	78,800
Salt Solubilities	mainly in water	ESLE	40,050
Azeotropic Data	in non-electrolyte systems	AZD	(60,150)
Partition Coefficients	octanol-water partition coefficients	KI	(15,050)
Adsorption Equilibria	vapor phase	AAE	5,850
Polymer Mixtures		POLYMER	22,800
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	24,450
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	7,400
Mixture Densities	includes also excess volumes	VE	85,850
Mixture Viscosities	includes also viscosity deviations	VIS	63,450
Thermal Conductivities (Mixtures)		MTCN	5,600
Surface Tensions (Mixtures)		MSFT	9,500
Flash Points of Flammable Liquid Mixtures		MFLP	1,020
Speeds of Sound (Mixtures)		MSOS	33,100
Dielectric constants (Mixtures)		MDEC	8,150
Gas Hydrates		GHD	5,700
Mixture PvT		MPVT	21,300
Mixture Electrical Conductivity		ECND	14,050
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	53,450

Dortmund Data Bank Modules, Pure Component Properties		Data Sets	Components
PCP-VAP+	Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	144,150	46,400
PCP-VIS+	Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	46,950	6,150
PCP-HCP+	Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	51,500	12,950
PCP-PVT+	Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	105,000	16,900
PCP-ENTH	Enthalpies of Combustion and Formation, several types of Entropies, Enthalpies, Energies	20,500	7,150
PCP-SFT	Surface Tensions	8,700	3,300
PCP-Other	Dielectric Constants, Diffusion Coefficients, Flash Points, Dipole Moments, Molar Polarization	9,900	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 Version	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	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(Ol).
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.