DDB

DDBST

Dortmund Data Bank
Software & Separation
Technology

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Product Overview 2024

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), 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.
Educational Version	This special version based on the *DDB Access Package* 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^∞, 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^∞, 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 *Predict Pure* 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^∞, 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, 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.

Product Overview 2024

Dortmund Data Bank Modules, Mixture Data			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	44,750
Vapor-Liquid Equilibria	low boiling substances	HPV	51,700
Vapor-Liquid Equilibria	electrolyte systems	ELE	15,500
Liquid-Liquid Equilibria		LLE	41,800
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(128,150)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	2,750
Gas Solubilities	in non-electrolyte systems	GLE	31,650
Gas Solubilities	in electrolyte systems	EGLE	5,000
Critical Data of Mixtures	critical lines	CRI	4,350
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	97,000
Salt Solubilities	in electrolyte systems	ESLE	53,400
Azeotropic Data	in non-electrolyte systems	AZD	(61,800)
Partition Coefficients	octanol-water partition coefficients	KI	(15,350)
Adsorption Equilibria	vapor phase	AAE	6,350
Polymer Mixtures		POLYMER	24,250
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	25,350
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	8,250
Mixture Densities	includes also excess volumes	VE	91,650
Mixture Viscosities	includes also viscosity deviations	VIS	74,700
Thermal Conductivities (Mixtures)		MTCN	6,350
Surface Tensions (Mixtures)		MSFT	11,550
Flash Points of Flammable Liquid Mixtures		MFLP	1,500
Speeds of Sound (Mixtures)		MSOS	41,400
Dielectric constants (Mixtures)		MDEC	8,750
Gas Hydrates		GHD	6,850
Mixture PvT		MPVT	24,700
Mixture Electrical Conductivity		ECND	21,300
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	79,650

Dortmund Data Bank Modules, Pure Component Properties		Data Sets	Components
PCP-VAP+	Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	179,000	63,850
PCP-VIS+	Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	49,600	6,750
PCP-HCP+	Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	74,700	20,250
PCP-PVT+	Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	113,000	18,800
PCP-ENTH	Enthalpies of Combustion and Formation, several types of Entropies, Enthalpies, Energies	23,650	8,450
PCP-SFT	Surface Tensions	9,250	3,500
PCP-Other	Dielectric Constants, Diffusion Coefficients, Flash Points, Dipole Moments, Molar Polarization	10,550	2,300

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(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.