DDBST
DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

DDB
Product Overview 2017

Phase Equilibria, Excess Properties, ….

Dortmund Data Bank*			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	38,695
Vapor-Liquid Equilibria	low boiling substances	HPV	41,090
Vapor-Liquid Equilibria	electrolyte systems	ELE	13,465
Liquid-Liquid Equilibria		LLE	32,475
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(96,390)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	1,770
Gas Solubilities	in non-electrolyte systems	GLE	24,140
Gas Solubilities	in electrolyte systems	EGLE	3,450
Critical Data of Mixtures	critical lines	CRI	3,360
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	60,270
Salt Solubilities	mainly in water	ESLE	41,910
Azeotropic Data	in non-electrolyte systems	AZD	(57,425)
Partition Coefficients	octanol-water partition coefficients	KI	(14,685)
Adsorption Equilibria	vapor phase	AAE	4,845
Polymer Mixtures		POLYMER	21,070
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	23,170
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	6,815
Mixture Densities	includes also excess volumes	VE	75,910
Mixture Viscosities	includes also viscosity deviations	VIS	44,795
Thermal Conductivities (Mixtures)		MTCN	4,825
Surface Tensions (Mixtures)		MSFT	6,215
Flash Points of Flammable Liquid Mixtures		MFLP	635
Speeds of Sound (Mixtures)		MSOS	20,465
Dielectric constants (Mixtures)		MDEC	7,285
Gas Hydrates		GHD	4,280
Mixture PvT		MPVT	14,455
Mixture Electrical Conductivity		ECND	9,955
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	32,225

Pure Component Properties

Dortmund Data Bank*	Data Sets	Components
Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	98,240	18,970
Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	38,600	4,030
Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	41,580	8,200
Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	87,710	10,370
Enthalpies of Combustion and Formation, Several Types of Entropies, Enthalpies, Energies	18,420	5,600
Surface Tensions	7,100	2,620
Further Thermophysical Properties	10,540	1,800
Pure Component Properties (1,928,000 data points, 302,230 data sets, 41,200 compounds)		

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.

*Changes and errors possible regarding all information.

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DDBSP
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Dortmund Data Bank Access Software*	
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 including complete data directory and demo versions of all non-licensed data banks.
+ 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.
+ Regression Mix Basic (1.4a) (Mixture Properties)	The regression add-on for mixture properties allows extended parameter fitting, calculation and graphical representation options for VLE, HPV, h^E, SLE and AZD with g^E models.
+ Regression Mix LLE (1.4b) (Liquid-Liquid Equilibria)	The regression add-on for liquid-liquid equilibria allows extended parameter fitting, calculation with g^E - models and provides graphical representation options.
+ 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 comp. 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).
++ GC-Parameters	Group interaction parameters for UNIFAC, mod. UNIFAC (Do) and PSRK developed during 20 years within the UNIFAC-Consortium are provided for mixture property estimation. Please visit http://www.unifac.org.

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) (group contribution estimation of pure component properties)	The world's leading 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 (100 different methods) including method quality estimation for several important properties.
+ Structures (2.2)	This add-on significantly enhances the ARTIST property estimation methods – providing molecular structures for more than 52,790 compounds.

Stand-Alone Software Tools*

Predictive GCEOS (2.3)	Prediction of vapor-liquid equilibria, gas solubilities, phase envelopes and SCF with VTPR and PSRK.
UNIFAC (2.4)	Enables the estimation of activity coefficients, h^E and c_P^E with UNIFAC and mod. UNIFAC (Do) 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 and does not require Predictive Methods (1.5).
Flash Point Estimation Via UNIFAC (2.6)	Enables the estimation of flash points of flammable liquid mixtures with UNIFAC and mod. UNIFAC (Do) for systems with up to 50 components. Flash Points for 965 components are included.

Upon Request*

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 single and multi-component adsorption on different adsorption agents with the help of 11 pure components (Freundlich, Langmuir, BET, Toth, ...) and 9 multi-component adsorption models (IAS, RAST, MIAS, ...).

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.

*Changes and errors possible regarding all information and prices. System requirements for version 2017: Official supported Microsoft Windows versions at release time.

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