

## Phase Equilibria, Excess Properties, ...

Dortmund Data Bank*			Data Sets (Data Points)
Vapor-Liquid Equilibria	normal boiling substances	VLE	40,500
Vapor-Liquid Equilibria	low boiling substances	HPV	44,600
Vapor-Liquid Equilibria	electrolyte systems	ELE	14,150
Liquid-Liquid Equilibria		LLE	35,450
Activity Coefficients	infinite dilution (in pure solvents)	ACT	(112,300)
Activity Coefficients	infinite dilution (in non-electrolyte mixtures)	ACM	2,000
Gas Solubilities	in non-electrolyte systems	GLE	26,600
Gas Solubilities	in electrolyte systems	EGLE	4,150
Critical Data of Mixtures	critical lines	CRI	3,450
Solid-Liquid Equilibria	mainly organic compounds, e.g. pharmaceuticals	SLE	68,650
Salt Solubilities	mainly in water	ESLE	44,500
Azeotropic Data	in non-electrolyte systems	AZD	(58,900)
Partition Coefficients	octanol-water partition coefficients	KI	(15,000)
Adsorption Equilibria	vapor phase	AAE	5,000
Polymer Mixtures		POLYMER	21,950
Excess Enthalpies	heats of mixing in non-electrolyte systems	HE	23,900
Heat Capacities of Mixtures	includes also excess heat capacities	CPE	7,100
Mixture Densities	includes also excess volumes	VE	80,900
Mixture Viscosities	includes also viscosity deviations	VIS	55,350
Thermal Conductivities (Mixtures)		MTCN	4,950
Surface Tensions (Mixtures)		MSFT	7,850
Flash Points of Flammable Liquid Mixtures		MFLP	730
Speeds of Sound (Mixtures)		MSOS	27,200
Dielectric constants (Mixtures)		MDEC	7,850
Gas Hydrates		GHD	5,150
Mixture PvT		MPVT	17,800
Mixture Electrical Conductivity		ECND	11,750
Miscellaneous Thermophysical Properties	diffusion coefficients, dissociation constants, etc.	X	46,100

## Pure Component Properties

Dortmund Data Bank*	Data Sets	Components
Vapor Pressures, Normal Boiling Points, Critical Data, Melting Points, Triple Points	130,700	42,000
Viscosities of Liquids, Vapors and Gases, Thermal Conductivities of Liquids and Vapors	44,700	5,800
Heat Capacities (solid, liquid, vapor, ideal gas), Heats and Entropies of Vaporization, Fusion and Transition	47,000	11,750
Liquid Densities, P-v-T Data, Virial Coefficients, Speed of Sound Data	97,950	15,500
Enthalpies of Combustion and Formation, Several Types of Entropies, Enthalpies, Energies	19,200	6,600
Surface Tensions	8,350	3,200
Further Thermophysical Properties	9,400	2,000
Pure Component Properties (> 2.07 million data points for more than 48,700 different compounds) basic price PC version: On request		

## 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.
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Basic pure component data files (1.2) for approximately 63,800 normal components, 9,100 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) are delivered with the VLE data bank.

\*Changes and errors possible regarding all information and prices.

Dortmund Data Bank Access Software*	
<b>Basic Version</b> (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.
<b>+ Regression Pure</b> (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.
<b>+ Regression Mix Basic</b> (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.
<b>+ Regression Mix LLE</b> (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.
<b>+ Predictive Methods</b> (1.5) (Mixture Properties)	The predictive methods UNIFAC, mod. UNIFAC (Do), ASOG, PSRK, VTPR, COSMO-SAC, COSMO-RS(OI) 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. $\sigma$ -profiles for 25 comp. and GC2GE (2.5)).
<b>++ <math>\sigma</math>-Profiles</b> (1.8) (COSMO-RS, COSMO-RS(OI))	A library of 4,435 $\sigma$ -profiles is provided for use with COSMO-SAC and COSMO-RS(OI).
<b>++ GC-Parameters</b>	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 <a href="http://www.unifac.org">http://www.unifac.org</a> .

## Dortmund Data Bank Advanced Packages\*

<b>RECPAR</b> (1.6a)	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>RECPAR EOS</b> (1.6b)	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> (1.7)	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> (1.9)	Selection of selective solvents by data bank access or using thermodynamic models.

## ARTIST Property Estimation Software\*

<b>Basic Version</b> (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.
<b>+ Structures</b> (2.2)	This add-on significantly enhances the ARTIST property estimation methods – providing molecular structures for more than 61,200 compounds.

## Stand-Alone Software Tools\*

<b>Predictive GCEOS</b> (2.3)	Prediction of vapor-liquid equilibria, gas solubilities, phase envelopes and SCF with VTPR and PSRK.
<b>UNIFAC</b> (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.
<b>GC2GE</b> (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 (OI)). GC2GE is included in 1.5 and does not require Predictive Methods (1.5).
<b>Flash Point Estimation Via UNIFAC</b> (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 1,220 components are included.

## Upon Request\*

<b>Educational Versions</b> (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.
<b>Vapor Phase Adsorption Software</b> (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.

<b>PCP Correlation Parameters</b>	Correlation parameters for pure component properties (e.g. Antoine-, Vogel- or DIPPR105 equation for 2000 – 5000 components)
<b>BIP's</b>	DDBST offers the fitting of binary interaction parameters to experimental data (e.g. NRTL, EOS, ...).
<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.

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