

DDB

Version 2025

Release Notes



DDBST - Dortmund Data Bank Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Phone: +49 441 361819 0

support@ddbst.com

www.ddbst.com

Contents

1	Installation notes	3
2	General	3
3	License Management	3
3.1	License Server	3
4	Dortmund Data Bank	3
5	Parameter DDB Organizer	3
6	Mixture Prediction	3
7	Regression Mix	4
8	Regression Pure	4
9	Miscellaneous	4
10	Dortmund Data Bank Progress (2025)	5
10.1	Overall Statistics	5
10.2	Pure Component Properties Data Bank Parts	6

1 Installation notes

The current software release can be installed in parallel to any previous release. However, if a previous release is uninstalled after the installation of the current release, then settings like the file type associations will get broken. In that case, a repair installation of the current release should solve the problem.

An officially supported Microsoft Windows version at release time is required.

2 General

- The databases have been updated to Firebird 5. For private databases, no upgrade is required.
- It is now possible to open .ddbpr files with double-click.
- The Excel export now supports *.xlsx files.

3 License Management

License are now provided as *.ddblic files. The file extension is now registered to install a license by double-click. The license server has to be updated to the latest version to be able to install the new license.

The license can also be installed by dragging it into the license management application.

3.1 License Server

The license server uses a new web server technology:

- The server does no longer use a password file. Existing accounts have to be created again. The default login is “admin” with the password “admin”.
- HTTPS is now always enabled. The server will generate a self-signed certificate (rlm-cert.pem) and key (rlm-key.pem) on startup, if they do not exist. These file are not removed on uninstall.

4 Dortmund Data Bank

- HPV and VLE data are displayed in one page in the query result window. They can be separated using a filter.
- The search result filters have been rewritten. It is possible to cumulate filters. Furthermore, temperature range and pressure range filters (where appropriate) have been introduced.
- Selected units are set for PCP and mixture data.
- The PCP search has been moved to a start window page.

5 Parameter DDB Organizer

Added support for creating new data sets.

6 Mixture Prediction

- Added support for AVEVA SimCentral.
- CalculateX3 does now support NRTL, UNIQUAC, Wilson.
- The “Predict Mix” plot has been improved.

- The phase envelope calculation now supports the UNIFAC Consortium versions of PSRK and VTPR. Furthermore, non-GC cubic EOS are now supported.
- Added support for [UNIFAC 2.0](#) and [Modified UNIFAC 2.0](#).

7 Regression Mix

- The GC2gE functionality has moved to the Regression Mix application.
- It is possible to add calculated data using GC models.
- Added support for AVEVA SimCentral.
- The Excel summary replaces the short summary.
- The DCDS fit supports multiple models.

8 Regression Pure

- Pressure and temperature depended liquid densities can be used to fit a Tait equation. The fitted Tait equation can calculate not only densities but also the Isothermal Compressibilities and Thermal Expansion Coefficients.

9 Miscellaneous

As usual, this release contains general bug fixes and performance improvements.

10 Dortmund Data Bank Progress (2025)

10.1 Overall Statistics

The Dortmund Data Bank 2025 contains more than 80,700 new data sets and more than 495,400 new data points.

DDB	2024		2025		Absolute Gain		Relative Gain	
	Sets	Points	Sets	Points	Sets	Points	Sets	Points
AAE	6350	88700	6750	95400	400	6700	6.30 %	7.55 %
ACM	2750	14600	2800	14900	50	300	1.82 %	2.05 %
ACT	128150	128100	128700	128700	550	600	0.43 %	0.47 %
AZD	61800	61800	62400	62400	600	600	0.97 %	0.97 %
CPE	8250	95000	8400	96700	150	1700	1.82 %	1.79 %
CRI	4350	25800	4400	26200	50	400	1.15 %	1.55 %
EGLE	5000	31400	5150	32300	150	900	3.00 %	2.87 %
ELE	15500	195900	15900	201000	400	5100	2.58 %	2.60 %
ESLE	53400	364500	55150	377000	1750	12500	3.28 %	3.43 %
GLE	31650	155300	33400	162900	1750	7600	5.53 %	4.89 %
HE	25350	366200	25550	368900	200	2700	0.79 %	0.74 %
HPV	51700	430400	53900	450300	2200	19900	4.26 %	4.62 %
LLE	41800	386900	43000	394800	1200	7900	2.87 %	2.04 %
PCP	423150	2428900	460000	2543800	36850	114900	8.71 %	4.73 %
POLYMER	24250	269100	24850	276800	600	7700	2.47 %	2.86 %
POW	15350	15300	15600	15600	250	300	1.63 %	1.96 %
SLE	97000	842100	101700	881800	4700	39700	4.85 %	4.71 %
VE	91650	1030500	92950	1045200	1300	14700	1.42 %	1.43 %
VLE	44750	642600	45650	652500	950	9900	2.13 %	1.54 %
ECND	21300	225400	24600	267000	3300	41600	15.49 %	18.46 %
GHD	6850	47100	7200	48900	350	1800	5.11 %	3.82 %
MDEC	8750	80300	9700	86300	950	6000	10.86 %	7.47 %
MFLP	1530	10100	1860	11800	330	1700	21.57 %	16.83 %
MPVT	24700	409800	27700	451700	3000	41900	12.15 %	10.22 %
MSFT	11550	118900	12550	126800	1000	7900	8.66 %	6.64 %
MSOS	41400	464700	44200	493300	2800	28600	6.76 %	6.15 %
MTCN	6350	59700	6750	63600	400	3900	6.30 %	6.53 %
VIS	74700	770300	79600	818100	4900	47800	6.56 %	6.21 %
X other	75050	679900	85750	754600	10700	74700	14.26 %	10.99 %
Total	1389700	10273900	1470400	10769300	80700	495400	5.81 %	4.82 %

Disclaimer:

Numbers presented may differ for a specific delivery because of corrections or other necessary changes.

The data base short terms are:

AAE: Adsorbent/Adsorptive equilibria – ACM: Activity coefficients at infinite dilution of a solute in a binary solvent – ACT: Activity coefficients at infinite dilution of a solute in a pure solvent – AZD: Azeotropic data points – CPE: Heat capacities and excess heat capacities – CRI: Critical data of mixtures – DIF: Diffusion coefficients – ECND: Electrical conductivities – EGLE: Gas solubilities in electrolyte-containing mixtures – ELE: Vapor-liquid equilibria of electrolyte-containing mixture – ESLE: Salt solubilities – GHD: Gas hydrate data – GLE: Gas solubilities (gas-liquid equilibria) – HE: excess enthalpies – HPV: Vapor-liquid equilibria (at least one component has a normal boiling point below 0°C) – LLE: Liquid-liquid equilibria (miscibility gaps) – MDEC: Mixture dielectric constants – MFLP: Mixture Flash Points – MPVT: Mixture P-v-T data – MSFT: Mixture surface tensions – MSOS: Mixture speeds of sound – MTCN: Mixture thermal conductivities – PCP: Pure component properties (several dozen different properties) – POLYMER: Polymer related data (VLE, LLE, etc.) – POW: Octanol-Water partition coefficients – SLE: Solid-liquid equilibria (solubilities) – VE: volumes, densities and excess volumes of mixtures – VIS: Mixture viscosities – VLE: Vapor-liquid equilibria (all components with a normal boiling point above 0°C) – X: Different thermodynamic properties.

10.2 Pure Component Properties Data Bank Parts

The PCP parts are defined as shown in the following table:

Partial DDB	Data Sets	Data Points	Components
PCP-VAP	195350	533700	73300
PCP-VIS	50500	405200	6900
PCP-HCP	79850	688800	21450
PCP-PVT	115700	831000	19300
PCP-ENTH	24400	89000	8600
PCP-SFT	9450	45000	3550
PCP-Other	10800	54100	2350

The packages contain these properties:

PCP-VAP: Vapor Pressure, Critical Data, Triple Point, Melting Point, Heat of Vaporization, Heat of Fusion, Boiling Point, Heat of Sublimation, Standard Heat of Vaporization, Standard Heat of Melting, Standard Heat of Sublimation, Freezing Point (Supercooled Liquid to Crystal/Solid only), Decomposition Temperature, Heat of Crystallization, Hypothetical Vapor Pressure (often pS(VL) of Solid Compounds)

PCP-VIS: Dynamic Viscosity, Kinematic Viscosity, Thermal Conductivity

PCP-HCP: Molar Heat Capacity (c_p), Heat of Vaporization, Heat of Fusion, Mass Heat Capacity, Enthalpy (H0), Enthalpy (H298), Enthalpy (H-H298/T), Enthalpy (H-H0/T), Transition Temperature, Heat of Transition, Molar Heat Capacity (c_v), Mass Heat Capacity (c_v), Ideal Gas Heat Capacity, Molar Saturation Heat Capacity, Heat of Sublimation, Entropy of Vaporization, Entropy of Fusion, Entropy of Transition, Entropy of Formation, Mass Saturation Heat Capacity, Gibbs Energy of Sublimation, Entropy of Sublimation, Standard Heat of Vaporization, Standard Heat of Melting, Standard Heat of Sublimation, Heat of Crystallization

PCP-PVT: Density, Virial Coefficients, Volume, P-v-T, Speed of Sound, Virial Coefficients (Berlin form), Thermal Expansion Coefficient, Compressibility (isothermal), Compressibility (isentropic), Compressibility Factor (isothermal), Compressibility Factor (isentropic), Joule-Thomson Coefficient (isenthalpic dT/dP), Compressibility (adiabatic)

PCP-ENTH: Entropy, Std. Heat of Combustion, Std. Heat of Formation, Gibbs Energy of Form./T, Gibbs Energy of Form., G function (G-G0)/T, Enthalpy (H298/T), Gibbs Energy, Gibbs Energy (G-G0), Gibbs Energy (G-G298), Enthalpy, Entropy (S-S0), Entropy (S-S298), G function (G-G298)/T

PCP-SFT: Surface Tension

PCP-Other: Dielectric Constant, Diffusion Coefficient, Flash Point, Dipole Moment, Molar Polarization