DDB and DDBSP

Delivery 2018

Changes and New Features

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1 Support for Process Simulation Tools

The support for the newest versions of the simulation tools from Aspen (Aspen Plus version 10), Honeywell (UniSim Design version R460), and SimSci (PRO/II version 10.1) has been added.

2 Mixture Predictions

2.1 PC-SAFT

A first implementation of PC-SAFT[1,2] ("Perturbed-Chain Statistical Associating Fluid Theory equation of state") can be used to predict VLE of binary mixtures. This model comes with several hundred pure component parameters and some parameters for binary mixtures.

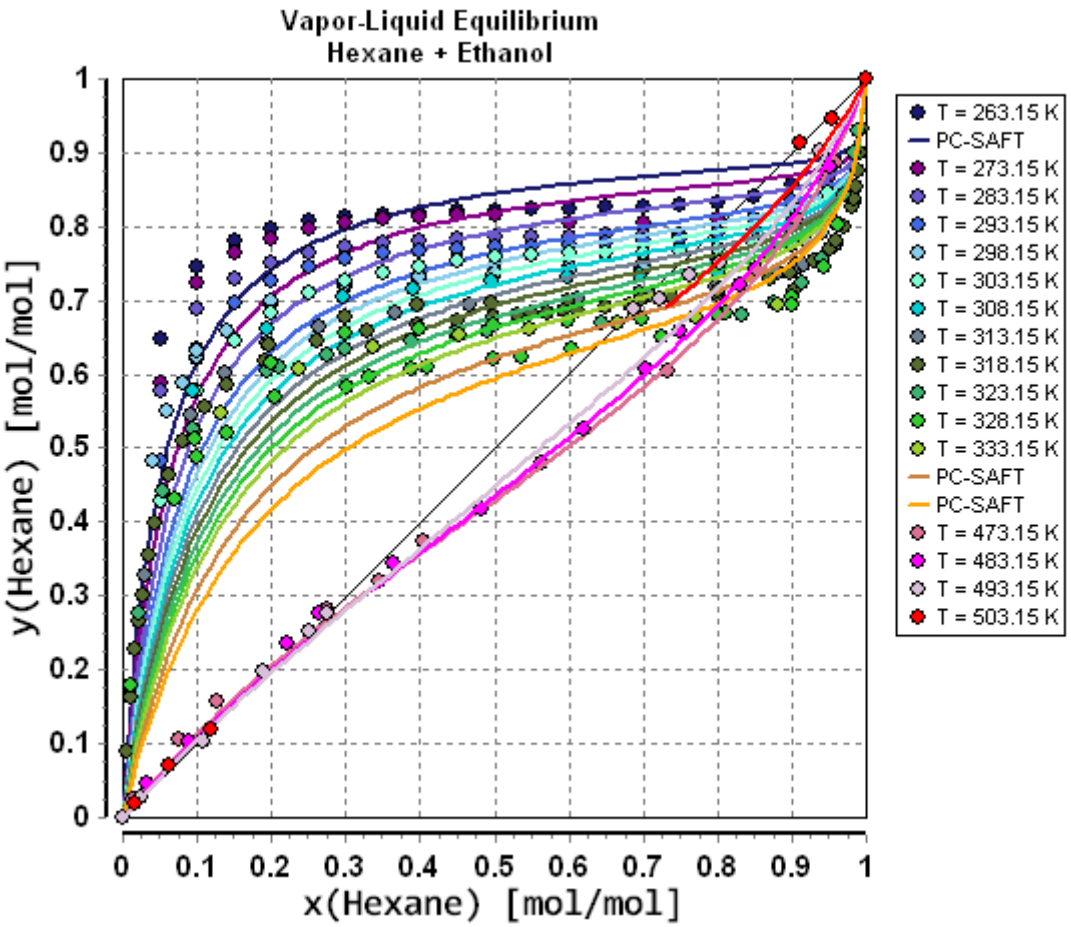


Figure 1: VLE Prediction for Ethanol/Hexane with PC-SAFT

1 Gross J.. Sadowski G.. "Perturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules". Ind.Eng.Chem.Res., 40(4), 1244-1260, 2001

2 Gross J.. Sadowski G.. "Application of the Pertubed-Chain SAFT Equation of State to Associating Systems". Ind.Eng.Chem.Res.. 41(22), 5510-5515, 2002

2.2 eNRTL

eNRTL[3,4,5,6] (short for electrolyte-NRTL) has be re-implemented and corrected and parameters have been updated. This implementation is now Aspen compatible and parameters can be exchanged.

2.3 Flash Point Predictions

The data base has been updated and the g^E models NRTL. Wilson. UNIQUAC have been added.

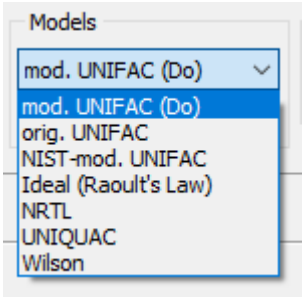


Figure 2: Flash Point Prediction - List of Models

The data bank now contains

- flash point temperatures for 1229 components (previously 965)
- heats of combustion for 1710 components (previously 1550)
- flash point temperatures and heats of combustion for 453 components (both needed values are available. previously 439)
- Antoine coefficients for approx. 6250 components (previously 5500)
- original UNIFAC group assignments for approx. 26750 components (previously 25.300)
- mod. UNIFAC (Dortmund) group assignments for approx. 30.850 components (previously 25.200)

2.4 SLE Predictions

Optional use of Neau[7] method

The calculation modes, either Schröder/van Laar or Neau, use slightly different equations for the determination of the solubilities.

Neau: $$\ln x_i = -\ln \gamma_i - \Delta_{fus} \frac{H}{RT_M} \ln\left(\frac{T_M}{T}\right)$$

Schröder/van Laar: $$\ln x_i = -\ln \gamma_i - \Delta_{fus} \frac{H}{R}\left(\frac{1}{T} - \frac{1}{T_M}\right)$$

3 Chen C.. Britt I.H.. Boston F.J.. Evans B.L.. "Local Composition Model for Excess Gibbs Energy of Electrolyte Systems. Part I: Single Solvent. Single Completely Dissociated Electrolyte Systems". AIChE J.. 28(4), 588-596, 1982

4 Mock B.. Evans B.L.. Chen C.-C.. "Thermodynamic Representation of Phase Equilibria of Mixed-Solvent Electrolyte Systems". AIChE J.. 32(10), 1655-1664, 1986

5 Chen C.-C.. Evans L.B.. "A Local Composition Model for the Excess Gibbs Energy of Aqueous Electrolyte Systems". AIChE J.. 32(3), 444-454, 1986

6 Chen C.-C.. Song Y.. "Generalized Electrolyte-NRTL Model for Mixed-Solvent Electrolyte Systems". AIChE J.. 50(8), 1928-1941, 2004

7 Neau S.H.. Bhandarkar S.V.. Hellmuth E.W.. "Differential Molar Heat Capacities to Test Ideal Solubility Estimations". Pharm.Res., 14(5), 601-605, 1997

2.5 Salt Solubility Prediction

Added prediction by UNIFAC (Kikic)[8] and eNRTL.

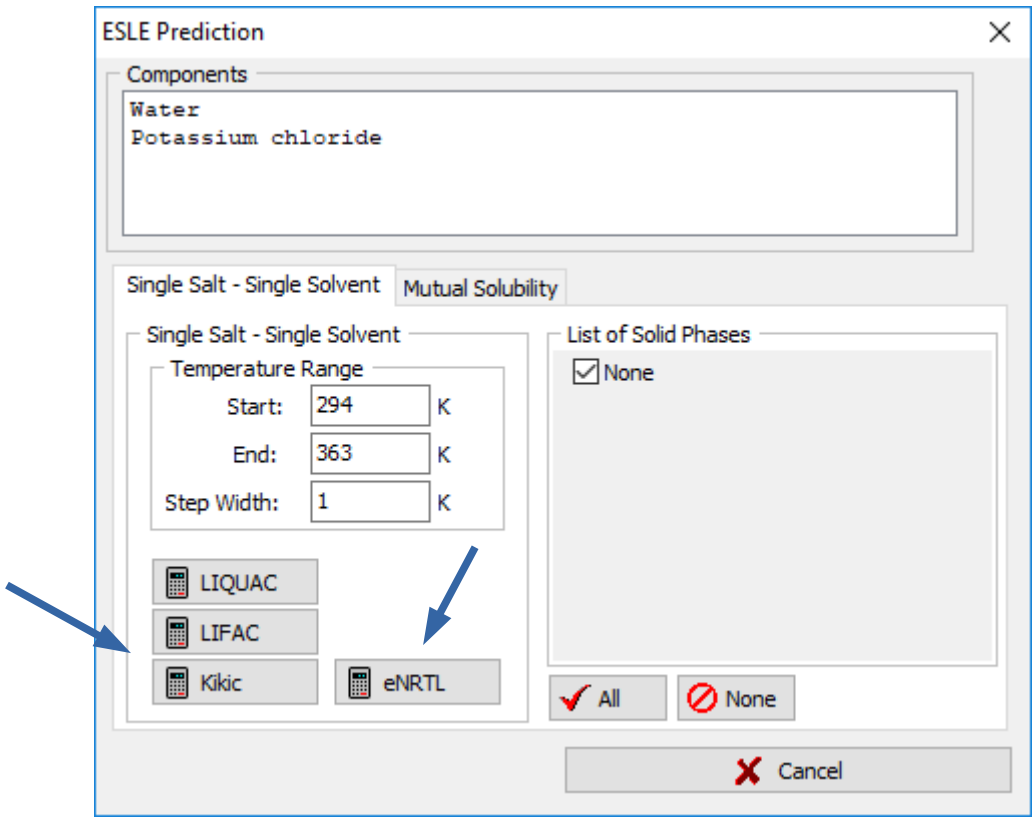


Figure 3: Salt Solubility Prediction

2.6 VLE Prediction

Prediction are now possible even without pure component vapor pressure equation. The pure component vapor pressure must then be given in experimental isothermal VLE data set.

2.7 Mixture Flash Points

Enabled prediction without previous selection of experimental data.

8 Kikic I.. Fermeglia M.. Rasmussen P.. "UNIFAC Prediction of Vapor-Liquid Equilibria in Mixed Solvent-Salt Systems". Chem.Eng.Sci., 46(11), 2775-2780, 1991

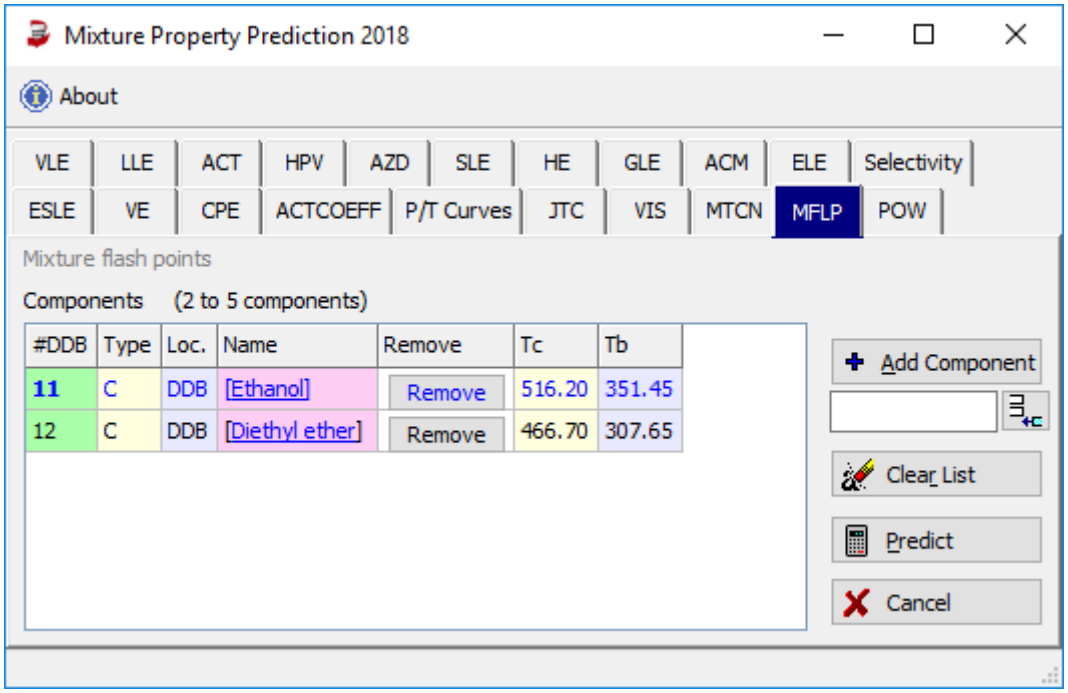


Figure 4: Direct Mixture Flash Point Prediction

2.8 Excess Heat Capacities and Enthalpies

Prediction with previously fitted parameters for Redlich-Kister and Sum of Symmetrical Functions is now possible.

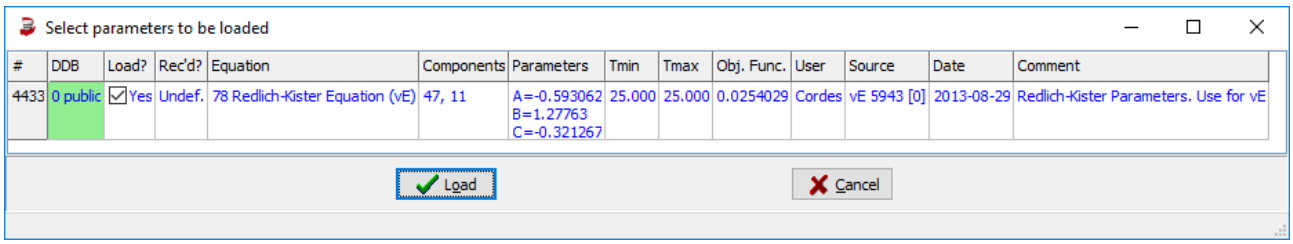


Figure 5: Redlich-Kister Parameter Selection

Also, mixing enthalpies can now be calculated with the COSMO-SAC Models 2010[9] and 2013[10].

9 Hsieh C.-M., Sandler S.I., Lin S.-T., "Improvements of COSMO-SAC for vapor-liquid and liquid-liquid equilibrium predictions", Fluid Phase Equilib., 297(1), 90-97, 2010

10 Hsieh C.-M., Lin S.-T., Vrabec J., "Considering the dispersive interactions in the COSMO-SAC model for more accurate predictions of fluid phase behavior", Fluid Phase Equilib., 367, 109-116, 2014

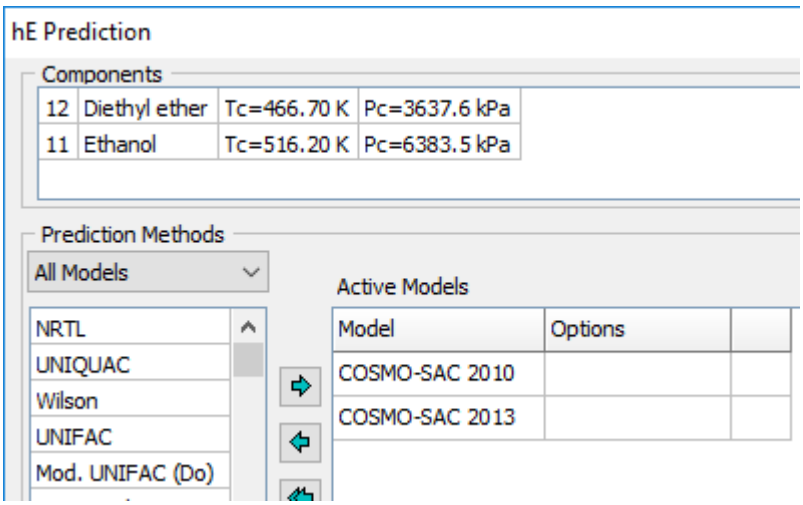


Figure 6: Prediction of Miing Enthalpies by COSMO-SAC 2010 and 2013

2.9 Critical Lines Prediction

It is now possible to start a critical line prediction from experimental CRIDDB data sets. Supported models are PSRK and VTPR.

The resulting diagram displays the predicted values together with the experimental data from the DDB.

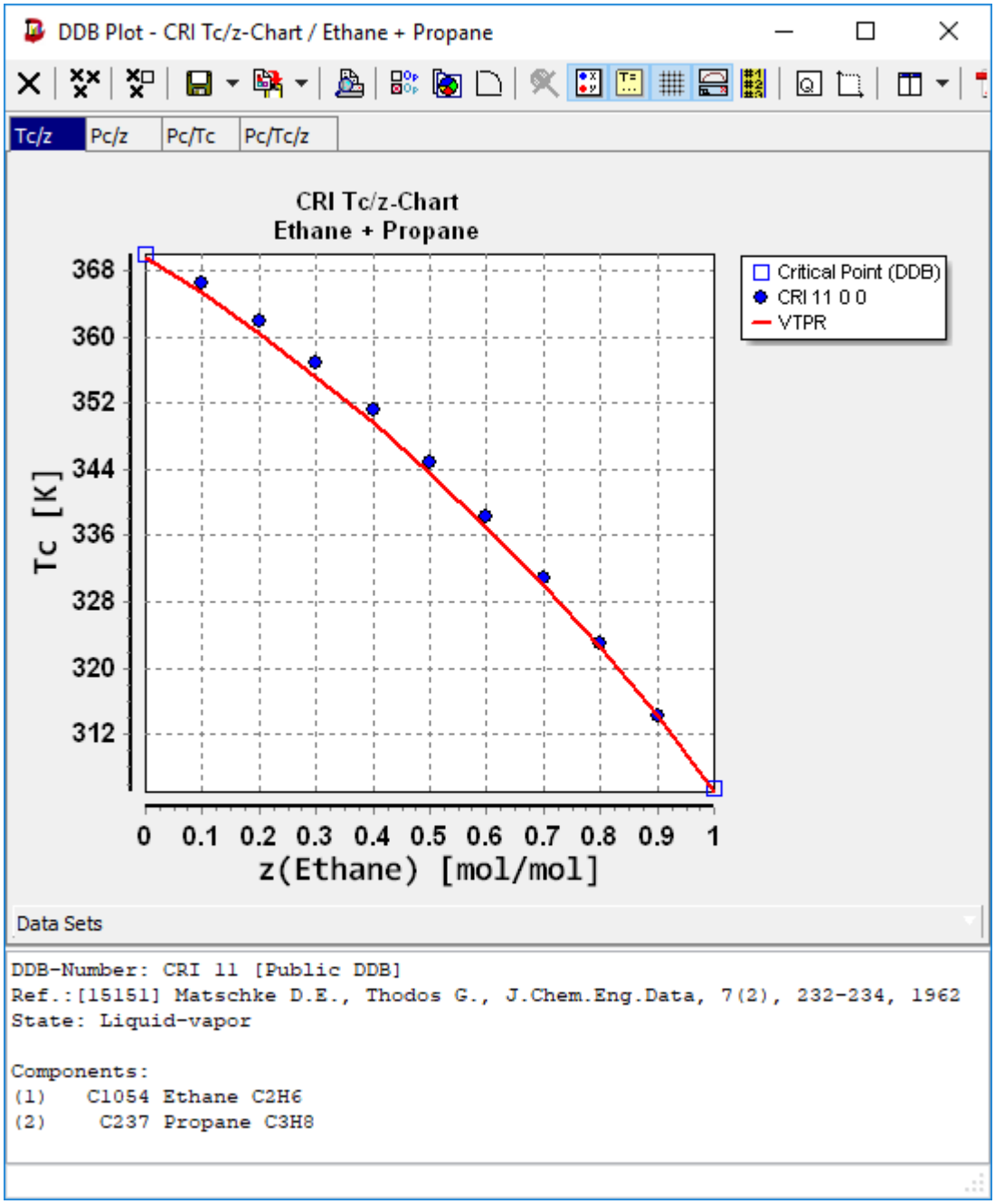


Figure 7: Critical Line Prediction

3 Installation and Setup

The installation is now MSI based. MSI stands for “Microsoft Installer” (now named “Windows Installer”) and is the standard format for setups in newer Windows versions. This format is directly supported by Microsoft and is guaranteed to be compatible with current and future versions of Windows operating systems. It needs no proprietary installer anymore, instead Windows provides the entire functionality.

4 Artist

4.1 Similarity Search

The similarity search is based on a group list and few other conditions like carbon count and number of branches.

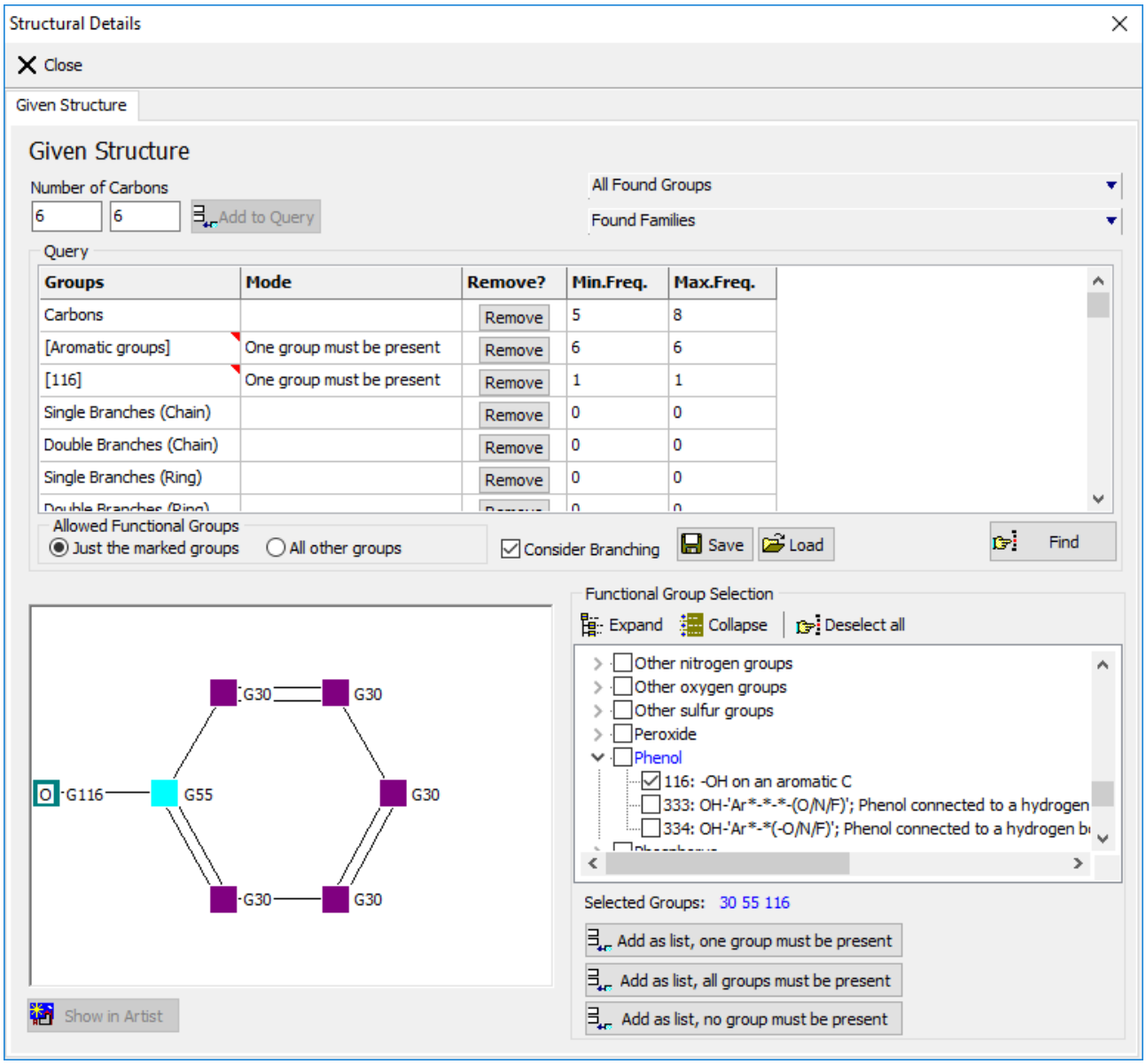


Figure 8: Similarity Search

4.2 Calculations

1. Additional pure component data are provided from DDB files (transition heats and temperatures)
2. Calculation of Octanol-Water partition coefficients at temperatures other than 25 °C

3. Added method of Hsu, Sheu, and Tu[11] for liquid dynamic viscosities.
4. Added method of Myers and Danner[12] for the prediction of ideal gas heat capacities

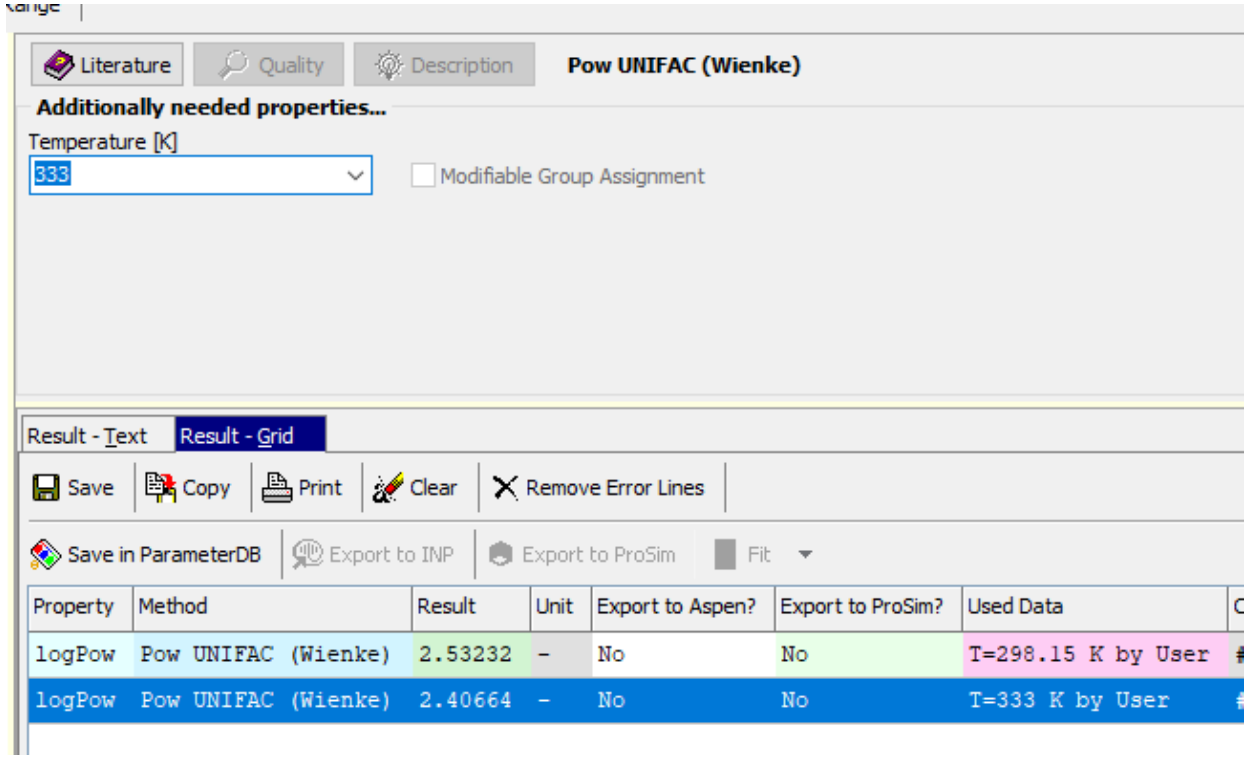


Figure 9: P_{OW} Calculation at Given Temperature

5 Pure Component Properties Equations

1. Support for Wilhoit equation (ideal gas heat capacities)

$$\frac{c_P}{R} = A + \left(\frac{B}{T^2}\right) \cdot \exp\left(\frac{-C}{T}\right) + D \cdot y^2 + \left(E - \frac{F}{(T-H)^2}\right) \cdot y^8 \quad \text{with} \quad y = \frac{T-G}{T+F}$$

2. Aly-Lee parameters (DIPPR 107) have been critically investigated and updated

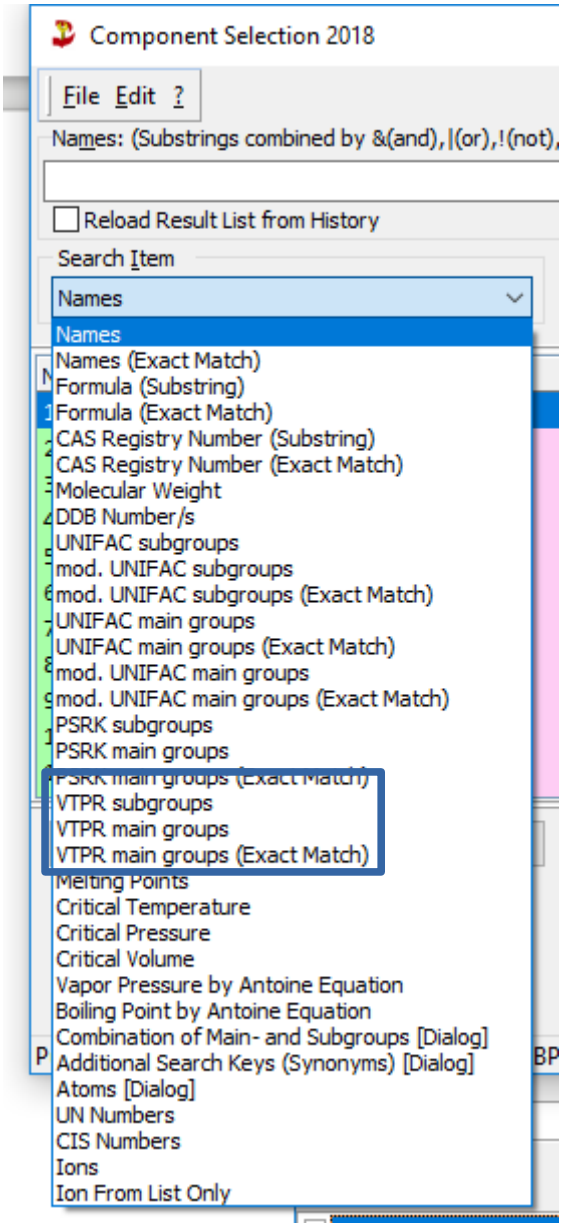
$$c_p = a_0 + a_1 \left(\frac{\frac{a_2}{T}}{\sinh\frac{a_2}{T}}\right)^2 + a_3 \left(\frac{\frac{a_4}{T}}{\cosh\frac{a_4}{T}}\right)^2$$

6 Component Selection

Search for VTPR groups added.

11 Hsu H.-C., Sheu Y.-W., Tu C.-H., "Viscosity Estimation at Low Temperatures (Tr < 0.75) for Organic Liquids from Group Contributions", Chem.Eng.J., 88, 27-35, 2002

12 Myers K.H., Danner R.P., "Prediction of Properties of Silicon, Boron, and Aluminum Compounds", J.Chem.Eng.Data, 38(2), 175-200, 1993



7 Literature Management

Multiple dialogs for editing data sets can now be opened simultaneously.

8 Pure Component Prediction

8.1 PSRK and VTPR

Prediction of heat capacity c_V for liquids and of heat of vaporization.

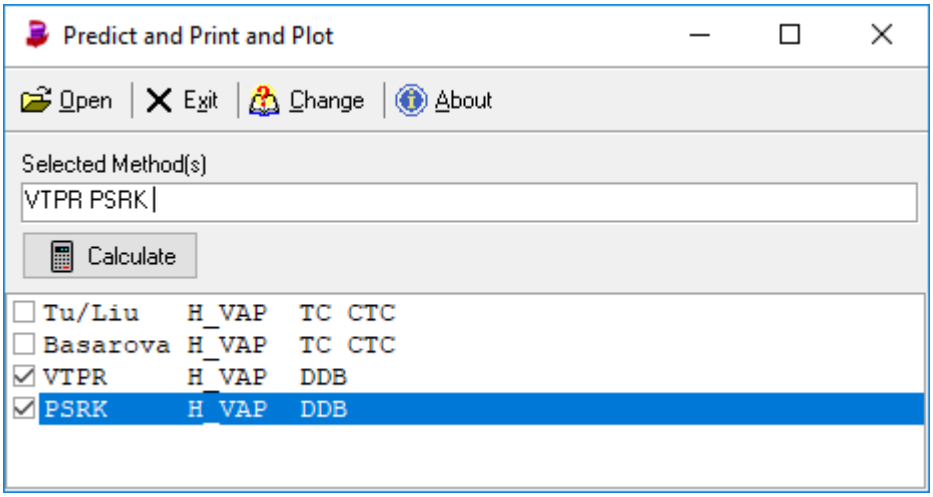


Figure 10: PSRK/VTPR Calculation of Heat of Vaporization

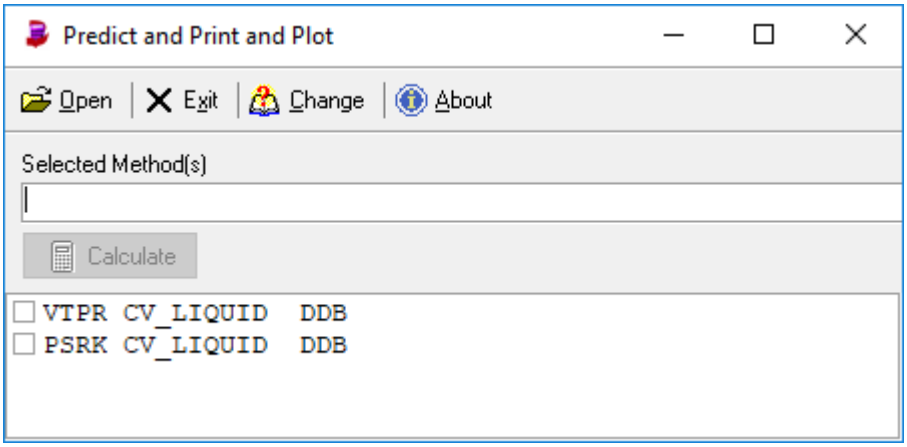


Figure 11: c_V Calculation with PSRK/VTPR

8.2 Equations with Parameters from ParameterDDB

Prediction of dielectric constants and liquid speed of sound by polynomial parameters.

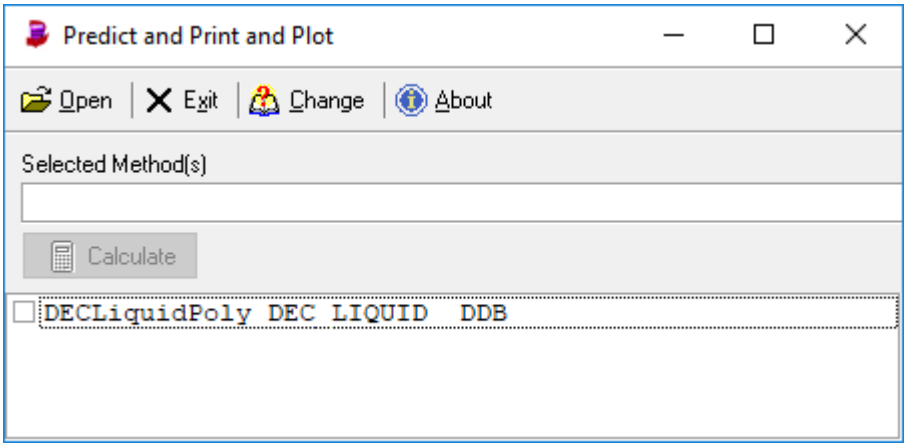


Figure 12: Dielectric Constants Calculation for Pure Component

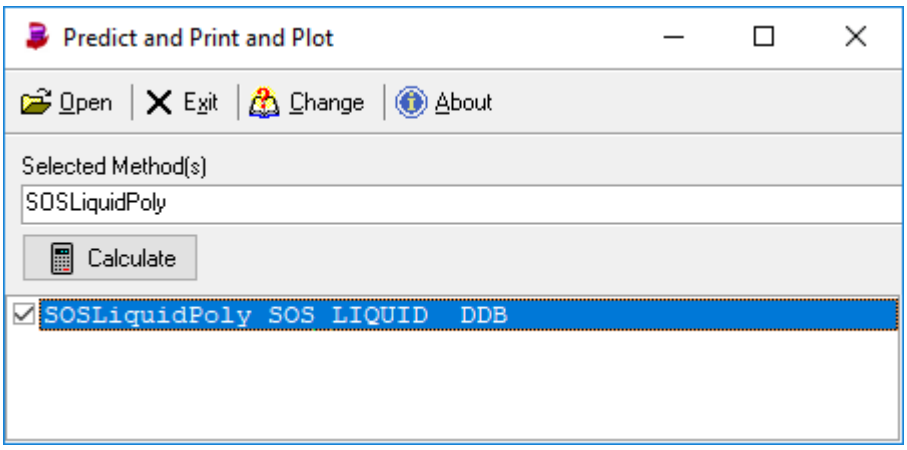
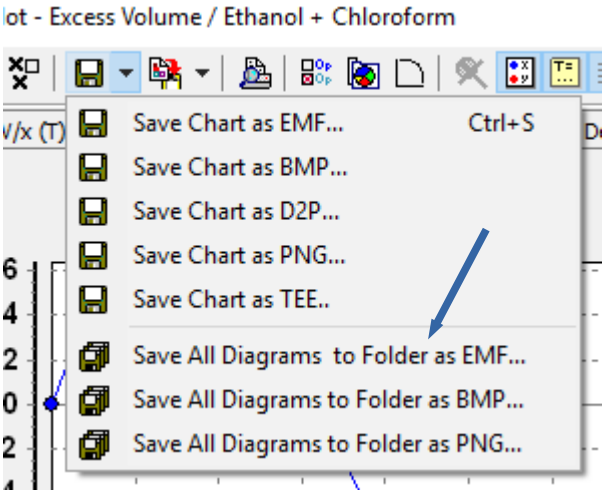


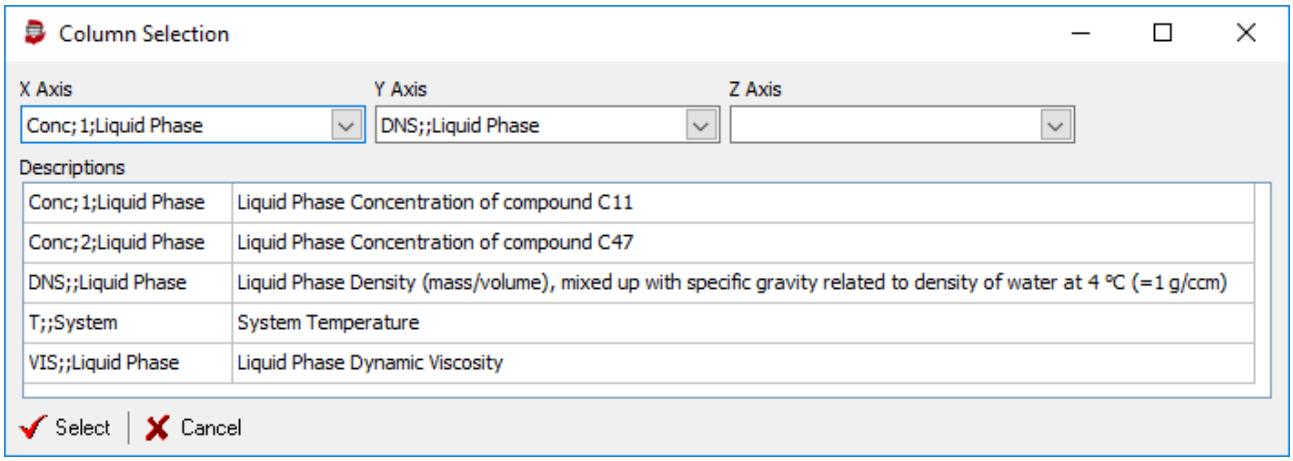
Figure 13: Speed of Sound Calculation for Pure Component

9 Plots

Enabled saving all diagrams in the different tabs of a single window:

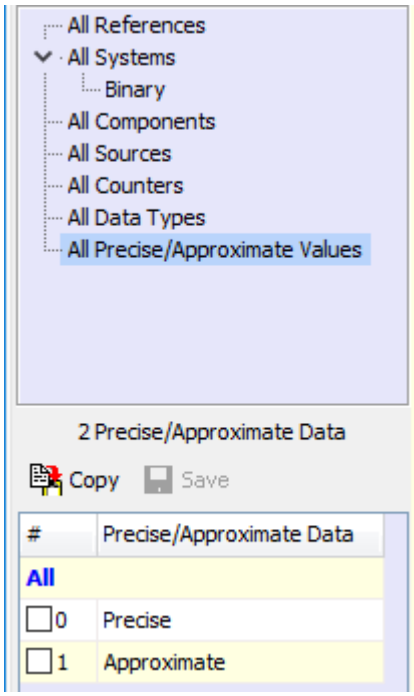


Added descriptions of short terms in XDDB column selection:

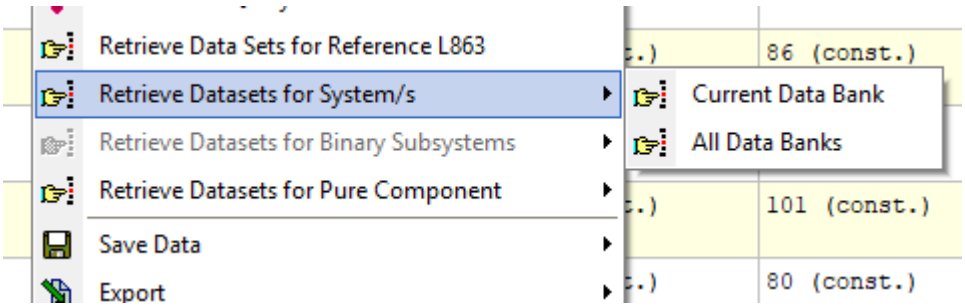


10 Data Handling in the Query Result

AZD Data: Mark data sets/points containing approximate values in query result



Allow searching data for current system in current data bank only.



11 Dortmund Data Bank Progress

11.1 Overall Statistics

The Dortmund Data Bank 2018 has more than 57000 new data sets and more than 405000 new data points. Data from more than 3400 sources have been added.

	2018			2017			Absolute Gain			Relative Gain		
Databank	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
AAE	5014	64052	309	4846	60645	295	+168	+3407	+14	3.47 %	5.62 %	4.75 %
ACM	1941	11080	87	1774	10599	83	+167	+481	+4	9.41 %	4.54 %	4.82 %
ACT	103139	103139	1449	96392	96392	1418	+6747	+6747	+31	7.00 %	7.00 %	2.19 %
AZD	58346	58346	8858	57427	57427	8684	+919	+919	+174	1.60 %	1.60 %	2.00 %
CPE	6977	80779	843	6819	78380	823	+158	+2399	+20	2.32 %	3.06 %	2.43 %
CRI	3420	23337	1079	3361	22975	1051	+59	+362	+28	1.76 %	1.58 %	2.66 %
DIF	2240	15302	399	2136	14757	370	+104	+545	+29	4.87 %	3.69 %	7.84 %
ECND	10575	110857	1002	9956	103690	927	+619	+7167	+75	6.22 %	6.91 %	8.09 %
EGLE	3979	24533	356	3450	19968	275	+529	+4565	+81	15.33 %	22.86 %	29.45 %
ELE	13807	173592	1924	13465	169308	1865	+342	+4284	+59	2.54 %	2.53 %	3.16 %
ESLE	42992	296266	7994	41911	289024	7798	+1081	+7242	+196	2.58 %	2.51 %	2.51 %
GHD	4795	34275	851	4281	31505	774	+514	+2770	+77	12.01 %	8.79 %	9.95 %
GLE	25996	124424	2613	24140	115492	2356	+1856	+8932	+257	7.69 %	7.73 %	10.91 %
HE	23696	346977	3418	23174	342613	3370	+522	+4364	+48	2.25 %	1.27 %	1.42 %
HPV	42610	365426	4874	41090	353411	4695	+1520	+12015	+179	3.70 %	3.40 %	3.81 %
LLE	34002	309335	5342	32479	293285	5084	+1523	+16050	+258	4.69 %	5.47 %	5.07 %
MDEC	7587	69533	941	7289	66887	885	+298	+2646	+56	4.09 %	3.96 %	6.33 %

	2018			2017			Absolute Gain			Relative Gain		
Databank	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
MFLP	713	5902	135	639	5381	121	+74	+521	+14	11.58 %	9.68 %	11.57 %
MPVT	16072	278991	1292	14457	253545	1177	+1615	+25446	+115	11.17 %	10.04 %	9.77 %
MSFT	7026	76789	852	6217	69251	772	+809	+7538	+80	13.01 %	10.89 %	10.36 %
MSOS	24137	288072	2180	20469	247558	1930	+3668	+40514	+250	17.92 %	16.37 %	12.95 %
MTCN	4866	43356	400	4828	42864	390	+38	+492	+10	0.79 %	1.15 %	2.56 %
PCP	317679	2001488	41792	302232	1928014	40086	+15447	+73474	+1706	5.11 %	3.81 %	4.26 %
POLYMER	21439	223142	1797	21072	219139	1758	+367	+4003	+39	1.74 %	1.83 %	2.22 %
POW	14883	14883	626	14686	14686	602	+197	+197	+24	1.34 %	1.34 %	3.99 %
SLE	64885	539457	9195	60270	496984	8715	+4615	+42473	+480	7.66 %	8.55 %	5.51 %
VE	79140	884313	8269	75911	851635	8000	+3229	+32678	+269	4.25 %	3.84 %	3.36 %
VIS	50165	523858	4588	44796	473077	4228	+5369	+50781	+360	11.99 %	10.73 %	8.51 %
VLE	39576	575626	8193	38696	562155	8015	+880	+13471	+178	2.27 %	2.40 %	2.22 %
X	36001	339508	4012	32226	310762	3549	+3775	+28746	+463	11.71 %	9.25 %	13.05 %
Sum	**1056639**	**7889238**	**81665**	**1001270**	**7500839**	**78210**	**+55369**	**+388399**	**+3455**	**+5.5 %**	**+5.2 %**	**+4.4 %**

Disclaimer: The numbers presented here may be different 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.

11.2 Pure Component Properties Data Bank Parts

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

Partial Data Bank	Components	Data Sets	Data Points
PCP-VAP+	38462	122792	406237
PCP-VIS+	5490	43179	335577
PCP-HCP+	11316	45132	492111
PCP-PVT+	14785	94692	685063
PCP-ENTH	6464	18715	74470
PCP-SFT	3073	7933	37963
PCP-Other	1981	9304	45135
Sum		341747	2076556
PCP Total	45075	317679	2001488
→ Overlap		24068	75068

The overlap is caused by some properties assigned to multiple packages and by some data sets containing multiple properties which might also be assigned to different packages.

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 (cP), 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 (cV), Mass Heat Capacity (cV), 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