

DDBSP 2018

Educational Version

Feature Matrix

DDBSP - Dortmund Data Bank Software Package



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	Educational Basic		Educational Professional		DDBSP Full Version	
Retrieval						
Search, table, plot, print, data export	•		•		•	
Prediction						
Predict g^E models (NRTL, Wilson, UNIQUAC)	○ ¹		•		•	
Predict group contribution (UNIFAC, Mod. UNIFAC (Dortmund), ASOG)	○ ¹		•		•	
Predict EOS (PSRK, VTPR)	○ ¹		•		•	
Predict COSMO-RS, COSMO-SAC	○ ¹		•		•	
Predict with Aspen (VLE, LLE, h^E , v^E , cp^E , γ^∞)	○ ¹		•		•	
Predict with PRO/II, UniSim Design, Simulis Thermodynamics (VLE, LLE)	○ ¹		•		•	
Flash EOS (PSRK, VTPR, several mixing rules)					•	
Regression						
Simple fit g^E – temperature independent (NRTL, Wilson, UNIQUAC)	•		•		•	
Fit EOS – temperature dependent (several mixing rules and alpha functions)	○ ²		○ ²		•	
Extended fit PCP			○ ³		•	
RecPar (simultaneous correlation of temperature dependent parameters for g^E models)	○ ⁴		○ ⁵		•	
Pure Component Property Estimation with Group Contribution (GC) Models from Structures						
Artist (structure editor)	•		•		•	
Structures (components)	750		56,900		56,900	
GC models / properties	27	24	27	24	103	52
Process Synthesis						
Azeotropic point prediction, contour lines, residual curves					•	
Entrainer Selection					•	
Private Data Management						
Literature	•		•		•	
Components, Structures	•		•		•	
Mixture / Pure Component Data			•		•	
Included Parameters						
Antoine Constants (components)	30		5,640		5,640	
Included Experimental Data (DDB)						
Pure Component Data (components)	30		30		45,000	
Data Sets (all properties)	81,300		81,300		1,056,500	
Data Points (all properties)	591,300		591,300		7,883,900	
Systems (all mixture properties)	1035		1035		153,900	

¹for the included 30 components only

²Redlich-Kwong EOS regression only

³for selected properties and equations including Wagner 2-5, DIPPR 101, 102, 104, 105 and 106

⁴3-Suffix-Margules regression only

⁵NRTL, Wilson, UNIQUAC regression only