

DDB Educational Version

2022

Feature Matrix



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	Educational Version		Full Version	
Retrieval				
Search, table, plot, print, data export	•		•	
Prediction				
Predict g^E models (NRTL, Wilson, UNIQUAC)	•		•	
Predict group contribution (UNIFAC, mod. UNIFAC (Dortmund))	•		•	
Predict EOS (PSRK, VTPR)	•		•	
Predict COSMO-RS, COSMO-SAC	•		•	
Predict with Aspen (VLE, LLE, h^E , v^E , cp^E , γ^∞)	•		•	
Predict with PRO/II, UniSim Design, Simulis Thermodynamics (VLE, LLE)	•		•	
Flash EOS (PSRK, VTPR, several mixing rules)			•	
Regression				
Regression Mix – parameter fitting for g^E models	○ ¹		•	
Regression Mix EOS – parameter fitting for cubic equations of state	○ ²		•	
Regression Mix Simulis – parameter fitting using Simulis Thermodynamics			•	
Extended PCP parameter fitting	○ ³		•	
Pure Component Property Estimation with Group Contribution (GC) Models from Structures				
Predict Pure (structure editor)	•		•	
Structures (components)	80,500+		80,500+	
GC models / properties	25+	20+	100+	50+
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)	6,500+		6,500+	
Included Experimental Data (DDB)				
Pure Component Data (components)	30		57,700+	
Data Sets (all properties)	86,000+		1,270,000+	
Data Points (all properties)	615,700+		9,500,000+	
Systems (all mixture properties)	1,000+		195,000+	

¹ NRTL, Wilson, UNIQUAC regression only

² Redlich-Kwong EOS regression only

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