

# DDB Educational Version

2025

## Feature Matrix



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	Educational Version		Full Version	
<b>Retrieval</b>				
Search, table, plot, print, data export	•		•	
<b>Prediction</b>				
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, Simulis Thermodynamics (VLE, LLE, AZD, $h^E$ , $v^E$ , $cp^E$ , $\gamma^\infty$ )	•		•	
Predict with PRO/II, UniSim Design (VLE, LLE)			•	
Flash EOS (PSRK, VTPR, several mixing rules)			•	
<b>Regression</b>				
Regression Mix – parameter fitting for $g^E$ models	○ <sup>1</sup>		•	
Regression Mix EOS – parameter fitting for cubic equations of state	○ <sup>2</sup>		•	
Regression Mix Simulis – parameter fitting using Simulis Thermodynamics			•	
Extended PCP parameter fitting	○ <sup>3</sup>		•	
<b>Pure Component Property Estimation with Group Contribution (GC) Models from Structures</b>				
Predict Pure (structure editor)	•		•	
Structures (components)	107,700+		107,700+	
GC models / properties	25+	20+	100+	50+
<b>Process Synthesis</b>				
Azeotropic point prediction, contour lines, residual curves			•	
Entrainer Selection			•	
<b>Private Data Management</b>				
Literature	•		•	
Components, Structures	•		•	
Mixture / Pure Component Data	•		•	
<b>Included Experimental Data (DDB)</b>				
Pure Component Data (components)	30		86,700+	
Data Sets (all properties)	94,500+		1,470,000+	
Data Points (all properties)	699,500+		10,769,000+	
Systems (all mixture properties)	1,300+		224,750+	

<sup>1</sup> NRTL, Wilson, UNIQUAC regression only

<sup>2</sup> Redlich-Kwong EOS regression only

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