

Ethyleneimine
151-56-4 | DTXSID8020599

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 9.93×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.26×10^{-1}

Confidence level: 5.66×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Ethyleneimine

Measured: 6.10×10^{-12}

Predicted: 9.93×10^{-12}

Image not found

Methanethiol

Measured: 3.29×10^{-11}

Predicted: 1.37×10^{-11}

Image not found

Ethanol

Measured: 3.27×10^{-12}

Predicted: 4.21×10^{-12}

Image not found

Dimethylamine

Measured: 6.54×10^{-11}

Predicted: 2.85×10^{-11}

Image not found

Ethanethiol

Measured: 4.68×10^{-11}

Predicted: 4.25×10^{-11}