

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.375

Global applicability domain: Inside

Local applicability domain index: 5.01e-01

Confidence level: 6.91e-01

Nearest Neighbors from the Training Set

Image not found

Ethylene oxide

Measured: -0.300

Predicted: -0.259

Image not found

1,2-Epoxy-3-fluoropropane

Measured: -0.160

Predicted: -0.152

Image not found

N-Methylethanolamine

Measured: -0.940

Predicted: -1.27

Image not found

2,2'-Bioxirane

Measured: -0.520

Predicted: -0.381

Image not found

1,2-Propylene oxide

Measured: 0.03

Predicted: 4.50e-02