

Ethylene oxide
75-21-8 | DTXSID0020600

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 18.1 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.55e-01

Confidence level: 6.76e-01

Nearest Neighbors from the Training Set

Image not found

Ethylene oxide

Measured: 22.7

Predicted: 18.1

Image not found

1,3-Propylene oxide

Measured: 17.2

Predicted: 11.1

Image not found

Dimethyl ether

Measured: 7.66

Predicted: 7.71

Image not found

1,2-Propylene oxide

Measured: 10.2

Predicted: 3.87

Image not found

Methylamine

Measured: 34.8

Predicted: 25.8