

Ethane
74-84-0 | DTXSID6026377

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: 3.58e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.69e-01

Confidence level: 6.97e-01

Nearest Neighbors from the Training Set

Image not found

Ethane

Measured: 2.00e-03

Predicted: 3.58e-03

Image not found

Ethylene

Measured: 4.67e-03

Predicted: 7.89e-03

Image not found

1-Propene

Measured: 4.75e-03

Predicted: 6.81e-03

Image not found

Propane

Measured: 1.42e-03

Predicted: 2.85e-03

Image not found

1-Propyne

Measured: 9.08e-02

Predicted: 6.74e-02