

Ethane
74-84-0 | DTXSID6026377

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.02

Global applicability domain: Inside

Local applicability domain index: 6.43e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Nitropropane

Measured: 8.32

Predicted: 7.41

[Image not found](#)

Furan

Measured: 5.01

Predicted: 4.88

[Image not found](#)

Thiophene

Measured: 8.91

Predicted: 6.68

[Image not found](#)

Diethyl ether

Measured: 5.37

Predicted: 4.72

[Image not found](#)

Carbon disulfide

Measured: 19.5

Predicted: 17.4