

Furan

110-00-9 | DTXSID6020646

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: 1.54 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.43e-01

Confidence level: 5.79e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Propylene oxide

Measured: 17.2

Predicted: 11.1

Image not found

Tetrahydrofuran

Measured: 13.9

Predicted: 2.96

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Methoxyethene

Measured: 2.58e-01

Predicted: 4.90e-01

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Ethene, 1,1'-oxybis-

Measured: 7.76e-02

Predicted: 2.49e-01

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1,2-Epoxybutane

Measured: 1.04

Predicted: 1.74