

Chloropicrin
76-06-2 | DTXSID0020315

Model Performance

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

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: 1.77e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.58e-01

Confidence level: 7.51e-01

Nearest Neighbors from the Training Set

Image not found

Chloropicrin

Measured: 9.86e-03

Predicted: 1.77e-02

Image not found

1,1-Dichloro-1-nitroethane

Measured: 1.74e-02

Predicted: 2.48e-02

Image not found

1-Chloro-2-nitropropane

Measured: 6.48e-02

Predicted: 3.89e-02

Image not found

Propane, 1,1-dichloro-1-nitro-

Measured: 3.17e-02

Predicted: 3.17e-02