

Chloromethane
74-87-3 | DTXSID0021541

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: -25.1 °C

Global applicability domain: Outside

Local applicability domain index: 5.49e-01

Confidence level: 6.69e-01

Nearest Neighbors from the Training Set

Image not found

Chloromethane

Measured: -24.0

Predicted: -25.1

Image not found

Ethane

Measured: -88.6

Predicted: -73.8

Image not found

Methyl bromide

Measured: 3.50

Predicted: 3.94

Image not found

Methanethiol

Measured: 5.90

Predicted: 7.36