

Chloropicrin
76-06-2 | DTXSID0020315

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -58.2 °C

Global applicability domain: Inside

Local applicability domain index: 4.08e-01

Confidence level: 5.67e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Chloropicrin

Measured: -64.0

Predicted: -58.2

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Bromopicrin

Measured: 10.0

Predicted: 4.58

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Ethene, nitro-

Measured: -55.5

Predicted: -62.1

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Nitromethane

Measured: -28.5

Predicted: -42.3

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Ethyl nitrate

Measured: -94.6

Predicted: -88.0