

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.65e-14 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.73e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

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Chloromethane

Measured: 4.36e-14

Predicted: 4.65e-14

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Methyl bromide

Measured: 4.02e-14

Predicted: 4.35e-14

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Dibromomethane

Measured: 1.13e-13

Predicted: 7.92e-14

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HFC-41

Measured: 1.68e-14

Predicted: 3.57e-14

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Bromochloromethane

Measured: 8.80e-14

Predicted: 7.28e-14