

Dibromomethane
74-95-3 | DTXSID4021557

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.12

Global applicability domain: Inside

Local applicability domain index: 9.89e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

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Dibromomethane

Measured: 3.07

Predicted: 3.12

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N,N-Dimethylformamide

Measured: 4.38

Predicted: 3.13

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Isopropyl ether

Measured: 2.66

Predicted: 2.82

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3-Methyl-2-butanone

Measured: 3.04

Predicted: 2.75

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1-Hexene

Measured: 2.41

Predicted: 2.75