

2-Bromo-1,1-dichloroethylene
5870-61-1 | DTXSID50207401

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: 3.59e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.05e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

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Trichloroethylene

Measured: 2.36e-12

Predicted: 2.21e-12

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(Z)-1,2-Dichloroethylene

Measured: 2.48e-12

Predicted: 2.80e-12

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(E)-1,2-Dichloroethylene

Measured: 2.48e-12

Predicted: 2.80e-12

Image not found

Oxazole

Measured: 9.10e-12

Predicted: 3.15e-11

Image not found

Chloral

Measured: 1.60e-12

Predicted: 1.64e-12

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Furan

Measured: 4.05e-11

Predicted: 3.25e-11