

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.98e-15 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.86e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

Image not found

Methane,
(difluoromethoxy)trifluoro-

Measured: 3.50e-15

Predicted: 4.56e-15

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1,2-Dibromo-1,1,2,2-
tetrafluoroethane

Measured: 1.30e-16

Predicted: 2.57e-16

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1,1,1,3,3,3-Hexafluoro-2-
propanol

Measured: 2.58e-14

Predicted: 2.03e-14

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2-(Difluoromethoxy)-1,1,1,3,3,3-
hexafluoropropane

Measured: 7.50e-14

Predicted: 3.74e-14