

Dichloroacetylene
7572-29-4 | DTXSID7020429

Model Performance

Model	Data
-------	------

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: 1.99e-13 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.30e-01

Confidence level: 6.13e-01

Nearest Neighbors from the Training Set

Image not found

Hexachlorobenzene

Measured: 2.70e-14

Predicted: 2.87e-12

Image not found

1,2,4-Trichlorobenzene

Measured: 5.50e-13

Predicted: 3.13e-11

Image not found

1,3,5-Triazine

Measured: 1.45e-13

Predicted: 3.40e-11

Image not found

Chloral

Measured: 1.60e-12

Predicted: 1.64e-12

Image not found

1,2-Dichlorobenzene

Measured: 4.20e-13

Predicted: 2.90e-11