

1,2,3,5-Tetrachlorobenzene
634-90-2 | DTXSID1026089

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: 3.29e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.46e-01

Confidence level: 5.66e-01

Nearest Neighbors from the Training Set

Image not found

Methylketene

Measured: 7.00e-11

Predicted: 6.39e-11

Image not found

Ethylketene

Measured: 1.18e-10

Predicted: 9.07e-11

Image not found

1,4-Naphthoquinone

Measured: 3.10e-12

Predicted: 3.16e-11

Image not found

Acenaphthylene

Measured: 1.10e-10

Predicted: 4.13e-11

Image not found

(Z)-Dichloropropene

Measured: 1.12e-11

Predicted: 1.42e-11

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trans-1,3-Dichloropropene

Measured: 1.12e-11

Predicted: 1.42e-11