

1,1,2,3-Tetrachloropropene
10436-39-2 | DTXSID2051475

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.70 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

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Methamidophos

Measured: 2.68

Predicted: 6.06e-05

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2,3-Dimethylbutane

Measured: 4.62

Predicted: 313

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Phoxim

Measured: 9.38e-01

Predicted: 1.27e-05

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Pentatriacontane

Measured: 12.0

Predicted: 8.42e-12

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1,1-Difluoro-2-methoxyethane

Measured: 77.2

Predicted: 511