

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 17.3 °C

Global applicability domain: Inside

Local applicability domain index: 7.13e-01

Confidence level: 3.77e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Butadiene, 1,2,3,4-tetrachloro-

Measured: -4.00

Predicted: 21.5

Image not found

Propane, 1,3-dibromo-2,2-bis(bromomethyl)-

Measured: 163

Predicted: 88.5

Image not found

Propane, 1,2,3-tribromo-

Measured: 16.9

Predicted: 8.98e-01

Image not found

Propane, 1,1,2,3,3-pentachloro-

Measured: -10.0

Predicted: -13.7

Image not found

Trichloroethylene

Measured: -84.7

Predicted: -59.8