

1,1,1,2-Tetrachloroethane
630-20-6 | DTXSID2021317

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 144 °C

Global applicability domain: Inside

Local applicability domain index: 7.73e-01

Confidence level: 7.36e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,1,1,2-Tetrachloroethane

Measured: 131

Predicted: 144

[Image not found](#)

1,1,2,2-Tetrachloroethane

Measured: 147

Predicted: 148

[Image not found](#)

1-Bromo-4-chlorobutane

Measured: 175

Predicted: 161

[Image not found](#)

1,2,3-Trichloropropane

Measured: 157

Predicted: 144