

1,2,3-Trichloropropene
96-19-5 | DTXSID3047766

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: 132 °C

Global applicability domain: Inside

Local applicability domain index: 9.44e-01

Confidence level: 7.06e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,2,3-Trichloropropene

Measured: 142

Predicted: 132

[Image not found](#)

1-Propene, 1,1,3-trichloro-

Measured: 132

Predicted: 132

[Image not found](#)

1-Propene, 1,1,2-trichloro-

Measured: 118

Predicted: 129

[Image not found](#)

1,4-Oxathiane

Measured: 147

Predicted: 138

[Image not found](#)

Ethanethioic acid, S-ethyl ester

Measured: 116

Predicted: 141

[Image not found](#)

Ethanethioic acid, S-ethyl ester

Measured: 116

Predicted: 141