

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 182 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.61e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

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1,1,2-Trichloroethane

Measured: 77.6

Predicted: 87.6

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Benzene, iodo-

Measured: 1260

Predicted: 1010

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1,1,1-Trichloroethane

Measured: 89.1

Predicted: 73.5

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Bromobenzene

Measured: 309

Predicted: 333

[Image not found](#)

1,3-Dichloropropene

Measured: 46.2

Predicted: 49.4

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trans-1,3-Dichloropropene

Measured: 46.2

Predicted: 49.4