

Hexachloroethane
67-72-1 | DTXSID7020689

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.38e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.18e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

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Hexachloropropene

Measured: 6.84e-05

Predicted: 2.12e-04

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1,2-Dibromo-3-chloropropane

Measured: 4.69e-03

Predicted: 2.20e-03

Image not found

Pentachloroethane

Measured: 2.37e-03

Predicted: 2.48e-03

Image not found

Benzene

Measured: 2.29e-02

Predicted: 1.13e-02

Image not found

Tetrachloroethylene

Measured: 1.21e-03

Predicted: 2.33e-03