

Hexachloropropene
1888-71-7 | DTXSID7062039

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.47

Global applicability domain: Outside

Local applicability domain index: 4.57e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

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Hexachloro-1,3-butadiene

Measured: 4.78

Predicted: 4.65

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Hexachloroethane

Measured: 4.14

Predicted: 4.00

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Hexachlorocyclopentadiene

Measured: 5.04

Predicted: 4.81

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Pentachloroethane

Measured: 3.22

Predicted: 3.19

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1,2,4,5-Tetrabromobenzene

Measured: 5.13

Predicted: 4.48