

Pentachloroethane
76-01-7 | DTXSID7021104

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: 3.19

Global applicability domain: Outside

Local applicability domain index: 4.20e-01

Confidence level: 6.23e-01

Nearest Neighbors from the Training Set

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Pentachloroethane

Measured: 3.22

Predicted: 3.19

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1,2-Dibromoethylene

Measured: 1.76

Predicted: 1.90

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Dibromomethane

Measured: 1.70

Predicted: 1.85

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Hexachlorocyclopentadiene

Measured: 5.04

Predicted: 4.81

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Hexachloroethane

Measured: 4.14

Predicted: 4.00