

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.00

Global applicability domain: Outside

Local applicability domain index: 4.01e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

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Hexachloroethane

Measured: 4.14

Predicted: 4.00

[Image not found](#)

Ethane, 1,2-diiodo-

Measured: 2.71

Predicted: 2.84

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Tribromoethene

Measured: 3.20

Predicted: 3.19

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Pentachloroethane

Measured: 3.22

Predicted: 3.19

[Image not found](#)

Hexachloro-1,3-butadiene

Measured: 4.78

Predicted: 4.65