

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.74e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.84e-01

Confidence level: 5.33e-01

Nearest Neighbors from the Training Set

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Dimethyl sulfoxide

Measured: 2.10e-01

Predicted: 3.98e-01

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1-Chloro-2-propanol

Measured: 18.5

Predicted: 5.24

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Phenyl carbonochloridate

Measured: 2.44e-01

Predicted: 1.81e-01

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Methyl isothiocyanate

Measured: 2.70e-01

Predicted: 5.52

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Dibromodifluoromethane

Measured: 39.0

Predicted: 781