

Chloral
75-87-6 | DTXSID7024744

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: 41.1 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.43e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

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2-Hydroxy-2-methylpropanenitrile

Measured: 50.0

Predicted: 3.02e-01

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1,1,2,2-Tetrachloroethane

Measured: 23.0

Predicted: 8.47

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2-Chlorobutane

Measured: 69.0

Predicted: 117

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2,2-Dimethylpropanoic acid

Measured: 3.50

Predicted: 5.74e-01

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Ethylene glycol

Measured: 255

Predicted: 4.90e-02