

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 30.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

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Trichloroacetic acid

Measured: 2.00

Predicted: 3.40

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Trichloroethylene

Measured: 100

Predicted: 83.1

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1,1,2,2-Tetrachloroethane

Measured: 79.4

Predicted: 77.8

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1,2-Dibromoethane

Measured: 51.3

Predicted: 55.8

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Chloropicrin

Measured: 61.7

Predicted: 61.7