

2-Chloroethanol
107-07-3 | DTXSID1021877

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: -0.00475

Global applicability domain: Inside

Local applicability domain index: 5.68e-01

Confidence level: 5.60e-01

Nearest Neighbors from the Training Set

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2-Chloroethanol

Measured: 0.03

Predicted: -0.00475

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3-Chloro-1-propanol

Measured: 0.5

Predicted: 5.74e-01

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Fluoroacetone

Measured: -0.390

Predicted: 1.41e-01

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2,3-Butanedione

Measured: -1.34

Predicted: -0.948

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Butyraldehyde

Measured: 0.88

Predicted: 7.87e-01