

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 7.71 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.61e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

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Thioacetamide

Measured: 6.03

Predicted: 6.43

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Methyl isothiocyanate

Measured: 9.33

Predicted: 7.63

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Epichlorohydrin

Measured: 10.0

Predicted: 9.87

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Pyridine

Measured: 39.8

Predicted: 20.1

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Acetic acid

Measured: 1.00

Predicted: 2.40