

Acetamide
60-35-5 | DTXSID7020005

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 19.0 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.62e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

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Acetamide

Measured: 38.1

Predicted: 19.0

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Acrylamide

Measured: 9.00

Predicted: 9.79

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Formamide

Measured: 22.2

Predicted: 16.8

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2-Fluoroacetamide

Measured: 13.0

Predicted: 12.6

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Bromoacetamide

Measured: 1.16

Predicted: 2.11