

Formyl chloride
2565-30-2 | DTXSID30180344

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: 2.01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.93e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

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Acrylonitrile

Measured: 1.40

Predicted: 1.84

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Chloroacetonitrile

Measured: 1.32

Predicted: 1.82

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Acetonitrile

Measured: 24.4

Predicted: 8.60

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Propionitrile

Measured: 1.87

Predicted: 1.77

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Methacrylonitrile

Measured: 3.79e-01

Predicted: 6.33e-01