

N,N-Dimethylformamide
68-12-2 | DTXSID6020515

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: 8.57 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.07e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

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N,N-Dimethylformamide

Measured: 13.7

Predicted: 8.57

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N,N-Dimethylacetamide

Measured: 11.5

Predicted: 8.06

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N-Nitrosomorpholine

Measured: 8.61

Predicted: 9.55

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Succinonitrile

Measured: 1.60

Predicted: 2.50

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Propanedinitrile

Measured: 2.01

Predicted: 2.19