

Acetaldehyde
75-07-0 | DTXSID5039224

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 1.79

Global applicability domain: Inside

Local applicability domain index: 9.60e-01

Confidence level: 6.06e-01

Nearest Neighbors from the Training Set

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Methyl formate

Measured: 1.75

Predicted: 1.78

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Acetonitrile

Measured: 2.31

Predicted: 1.96

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Propane

Measured: 0.97

Predicted: 1.60

[Image not found](#)

Nitromethane

Measured: 2.53

Predicted: 1.63

[Image not found](#)

Dimethyl ether

Measured: 1.37

Predicted: 1.58