

Methyl formate
107-31-3 | DTXSID5025609

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 36.7 °C

Global applicability domain: Inside

Local applicability domain index: 7.12e-01

Confidence level: 8.07e-01

Nearest Neighbors from the Training Set

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Methyl formate

Measured: 31.7

Predicted: 36.7

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Acetone

Measured: 55.8

Predicted: 48.2

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(2H6)Acetone

Measured: 55.8

Predicted: 50.0

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Propanal

Measured: 48.0

Predicted: 47.1

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Dimethoxymethane

Measured: 42.0

Predicted: 49.8