

Methanol
67-56-1 | DTXSID2021731

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.606

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

Image not found

Methanol

Measured: -0.770

Predicted: -0.606

Image not found

Methylamine

Measured: -0.570

Predicted: -0.633

Image not found

Methyl formate

Measured: 0.03

Predicted: -0.0580

Image not found

HFC-41

Measured: 0.51

Predicted: 3.18e-01

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2-Fluoroethanol

Measured: -0.670

Predicted: -0.450