

1-Pentanol
71-41-0 | DTXSID6021741

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: 3.20e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.58e-01

Confidence level: 9.20e-01

Nearest Neighbors from the Training Set

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1-Pentanol

Measured: 2.50e-01

Predicted: 3.20e-01

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Isopentyl alcohol

Measured: 3.03e-01

Predicted: 3.29e-01

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2-Methyl-1-butanol

Measured: 3.37e-01

Predicted: 3.41e-01

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Pent-4-en-1-ol

Measured: 6.62e-01

Predicted: 5.01e-01

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2,2-Dimethylpropanol

Measured: 3.97e-01

Predicted: 4.03e-01