

Isopentyl alcohol
123-51-3 | DTXSID3025469

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: 1.24

Global applicability domain: Inside

Local applicability domain index: 8.08e-01

Confidence level: 8.47e-01

Nearest Neighbors from the Training Set

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Isopentyl alcohol

Measured: 1.16

Predicted: 1.24

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2-Methyl-1-butanol

Measured: 1.29

Predicted: 1.26

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3-Pentanol

Measured: 1.21

Predicted: 1.21

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1-Pentanol

Measured: 1.51

Predicted: 1.36

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Pentan-2-ol

Measured: 1.19

Predicted: 1.21