

Propan-2-(¹⁷O)ol
1173018-27-3 | DTXSID30745952

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: 2.58e-01

Global applicability domain: Inside

Local applicability domain index: 6.45e-01

Confidence level: 7.38e-01

Nearest Neighbors from the Training Set

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Isopropanol

Measured: 0.05

Predicted: 2.58e-01

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1-Propanol

Measured: 0.25

Predicted: 1.27e-01

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2-Butanol

Measured: 0.61

Predicted: 7.73e-01

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1-Butanol

Measured: 0.88

Predicted: 8.38e-01

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2-Methyl-1-propanol

Measured: 0.76

Predicted: 8.81e-01