

1-Butanol
71-36-3 | DTXSID1021740

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.06e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.36e-01

Confidence level: 7.91e-01

Nearest Neighbors from the Training Set

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1-Butanol

Measured: 8.57e-12

Predicted: 1.06e-11

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2-Butanol

Measured: 9.60e-12

Predicted: 8.64e-12

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Cyclopentanol

Measured: 1.07e-11

Predicted: 1.17e-11

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1,4-Diazabicyclo[2.2.2]octane

Measured: 2.20e-11

Predicted: 1.30e-11

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1-Pentanol

Measured: 1.11e-11

Predicted: 1.18e-11