

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.92

Global applicability domain: Inside

Local applicability domain index: 5.38e-01

Confidence level: 7.28e-01

Nearest Neighbors from the Training Set

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Piperidine, 1-methyl-

Measured: 4.47

Predicted: 5.88

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Diethyl ether

Measured: 5.37

Predicted: 4.72

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2-Aminopyridine

Measured: 11.5

Predicted: 3.44

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cis-Nanophine

Measured: 5.01

Predicted: 6.12

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3-Pyridinamine

Measured: 2.09

Predicted: 3.04