

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.03

Global applicability domain: Inside

Local applicability domain index: 9.70e-01

Confidence level: 7.52e-01

Nearest Neighbors from the Training Set

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1-Butanol

Measured: 4.19

Predicted: 4.03

Image not found

Pyrrolidine

Measured: 4.07

Predicted: 4.10

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Butylamine

Measured: 3.61

Predicted: 4.09

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2-Chloroethanol

Measured: 4.30

Predicted: 4.07

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2-Methyl-1-propanol

Measured: 3.93

Predicted: 3.95