

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.88 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.27e-01

Confidence level: 8.34e-01

Nearest Neighbors from the Training Set

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Barbituric acid

Measured: 6.70

Predicted: 4.85e-08

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1-Propanol

Measured: 2.20

Predicted: 21.3

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Isobutylamine

Measured: 10.4

Predicted: 172

Image not found

Salicylic acid

Measured: 21.0

Predicted: 2.08e-05

Image not found

2,2-Dimethylbutane

Measured: 16.0

Predicted: 225