

2-Butanol
78-92-2 | DTXSID9021762

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: 12.0 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.28e-01

Confidence level: 7.45e-01

Nearest Neighbors from the Training Set

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2-Chloropropan-1-ol

Measured: 18.3

Predicted: 4.93

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Isobutylamine

Measured: 10.4

Predicted: 172

[Image not found](#)

Diacetone alcohol

Measured: 2.37

Predicted: 1.27

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Cyclohexane, tridecyl-

Measured: 6.11

Predicted: 9.77e-06

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Bromotrifluoromethane

Measured: 40.7

Predicted: 6290