

2-Butanol
78-92-2 | DTXSID9021762

Model Performance

Model	Data
-------	------

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: 5.21

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 8.27e-01

Nearest Neighbors from the Training Set

[Image not found](#)

tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

[Image not found](#)

Piperidine, 1-methyl-

Measured: 4.47

Predicted: 5.88

[Image not found](#)

Diethyl ether

Measured: 5.37

Predicted: 4.72

[Image not found](#)

4-Hydroxybenzonitrile

Measured: 8.13

Predicted: 4.19

[Image not found](#)

Dimethyl sulfoxide

Measured: 3.98

Predicted: 4.07