

Butyl 2-hydroxy-2-methylpropanoate
816-50-2 | DTXSID50278111

Model Performance

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

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: 4.70e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 5.64e-01

Nearest Neighbors from the Training Set

Image not found

1-Naphthylamine

Measured: 4.00e-01

Predicted: 9.37e-04

Image not found

Ethyl isobutyrate

Measured: 3.75

Predicted: 19.3

Image not found

2-Butanone, 1-bromo-

Measured: 1.26e-01

Predicted: 7.89

Image not found

Ethyl chloroacetate

Measured: 9.05e-01

Predicted: 7.43

Image not found

Nonylamine

Measured: 1.55e-01

Predicted: 2.75e-01