

2,2-Dimethylpropane-1,3-diol
126-30-7 | DTXSID8027036

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 18.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Diethylhydrazine

Measured: 15.1

Predicted: 14.1

Image not found

1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

Image not found

Butylamine

Measured: 75.9

Predicted: 19.9

Image not found

1-Butanol

Measured: 3.16

Predicted: 8.95