

Dimethyl sulfoxide
67-68-5 | DTXSID2021735

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.77 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.54e-01

Confidence level: 6.25e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Dimethyl sulfoxide

Measured: 12.8

Predicted: 8.77

[Image not found](#)

Acetone

Measured: 17.2

Predicted: 6.59

[Image not found](#)

Glyoxal

Measured: 17.2

Predicted: 13.1

[Image not found](#)

2,4-Pentanedione

Measured: 1.66

Predicted: 1.64