

2-Nitropropane
79-46-9 | DTXSID6020981

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.26

Global applicability domain: Inside

Local applicability domain index: 9.87e-01

Confidence level: 7.85e-01

Nearest Neighbors from the Training Set

Image not found

Isoprene

Measured: 2.06

Predicted: 2.26

Image not found

Carbon disulfide

Measured: 2.28

Predicted: 2.26

Image not found

Propionitrile

Measured: 2.69

Predicted: 2.26

Image not found

Methyl iodide

Measured: 2.16

Predicted: 2.26

Image not found

Bromoethane

Measured: 2.11

Predicted: 2.26