

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 12.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.67e-01

Confidence level: 6.53e-01

Nearest Neighbors from the Training Set

Image not found

Pyridine

Measured: 39.8

Predicted: 20.1

Image not found

Benzene

Measured: 56.2

Predicted: 50.5

Image not found

Epichlorohydrin

Measured: 10.0

Predicted: 9.87

Image not found

1-Propanol

Measured: 3.02

Predicted: 4.69

Image not found

1-Butanol

Measured: 3.16

Predicted: 8.95