

2-Isopropyl-6-methyl-4-pyrimidone
2814-20-2 | DTXSID1027502

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: 7.52e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 4.68e-01

Nearest Neighbors from the Training Set

Image not found

2-

Cyclohexylidenehydrazinecarboxamide

Measured: 3.87e-02

Predicted: 8.20e-02

Image not found

Thionicotinic acid

Measured: 4.17e-02

Predicted: 1.02e-01

Image not found

Quinoxalin-5(1H)-one

Measured: 4.50e-02

Predicted: 9.62e-02

Image not found

Glycine, N-benzoyl-, methyl ester

Measured: 8.80e-02

Predicted: 2.38e-02