

2-Amino-1-naphthalenesulfonic acid
81-16-3 | DTXSID7020922

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: 8.39

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.48e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Hydroxybenzoic acid

Measured: 8.08

Predicted: 7.78

[Image not found](#)

Salicylic acid

Measured: 7.44

Predicted: 7.60

[Image not found](#)

1-Hexadecanol

Measured: 9.90

Predicted: 9.79

[Image not found](#)

1-Octadecanol

Measured: 10.9

Predicted: 10.5

[Image not found](#)

Diphenylamine

Measured: 7.64

Predicted: 8.73