

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

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 2.78 days

Global applicability domain: Outside

Local applicability domain index: 4.20e-01

Confidence level: 8.98e-01

Nearest Neighbors from the Training Set

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Indene

Measured: 12.5

Predicted: 7.90

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3-Methylindene

Measured: 12.5

Predicted: 2.76

[Image not found](#)

1H-Indene, 2-methyl-

Measured: 12.5

Predicted: 2.48

[Image not found](#)

4-Methylindan

Measured: 4.93

Predicted: 2.31

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2-Ethyl-p-xylene

Measured: 12.5

Predicted: 3.70