

3-Amino-3-(naphthalen-1-yl)propanoic acid
100393-41-7 | DTXSID80377489

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.88e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 3.05e-01

Nearest Neighbors from the Training Set

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Naphthalene, 1,2,4,7-tetrachloro-

Measured: 3.45e-10

Predicted: 1.23e-05

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Methylcyclopentane

Measured: 9.75e-11

Predicted: 80.1

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2-Phenylcyclohexanol

Measured: 2.69e-06

Predicted: 1.03e-02

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Fenuron

Measured: 1.21e-05

Predicted: 1.82e-05

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Hydroprene

Measured: 3.39e-09

Predicted: 8.80e-04