

4-Amino-1-naphthalenesulfonic acid sodium salt
130-13-2 | DTXSID0059611

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.27e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.59e-01

Confidence level: 5.73e-01

Nearest Neighbors from the Training Set

Image not found

Dibenzofuran-2-sulphonic acid

Measured: 3.42e-01

Predicted: 4.46e-01

Image not found

4-Aminobenzenesulfonic acid

Measured: 6.24e-02

Predicted: 1.78e-01

Image not found

Benzenesulfonic acid, 3-amino-4-methoxy-

Measured: 1.26e-01

Predicted: 1.74e-01

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Benzenesulfonic acid, 3-hydrazino-

Measured: 1.49e-01

Predicted: 5.98e-01