

4-Hydroxy-1-naphthalenesulfonic acid monosodium salt
6099-57-6 | DTXSID6064113

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: 5.03e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.37e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

Image not found

Naphthalene-2-sulfonic acid

Measured: 3.26

Predicted: 1.08

Image not found

4-Aminobenzenesulfonic acid

Measured: 6.24e-02

Predicted: 1.78e-01

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Benzoic acid, 2-sulfo-

Measured: 2.47

Predicted: 1.38

Image not found

Phosphonic acid, (3-nitrophenyl)-

Measured: 4.83

Predicted: 1.16