

Aminotrimethylene phosphonic acid
6419-19-8 | DTXSID2027624

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.05

Global applicability domain: Outside

Local applicability domain index: 6.89e-02

Confidence level: 8.29e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Amino-5-hydroxy-2,7-naphthalenedisulfonic acid monosodium salt

Measured: 2.88

Predicted: 2.48

[Image not found](#)

7,7'-(Carbonyldiimino)bis[4-hydroxy-2-naphthalenesulfonic acid]

Measured: 1.82

Predicted: 2.69

[Image not found](#)

2,5-Pyridinedicarboxylic acid

Measured: 5.75

Predicted: 4.09

[Image not found](#)

3-Nitrophthalic acid

Measured: 5.25

Predicted: 4.93