

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -3.42

Global applicability domain: Outside

Local applicability domain index: 2.35e-01

Confidence level: 4.48e-01

Nearest Neighbors from the Training Set

Image not found

Aminotrimethylene phosphonic acid

Measured: -3.53

Predicted: -3.42

Image not found

Phosphonic acid, [1,6-hexanediylbis[nitrilobis(methylene)]tetra-

Measured: -4.43

Predicted: -4.25

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Cephacetrile

Measured: -0.450

Predicted: -0.464

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5-Acetamido-N¹,N³-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-N¹-methylbenzene-1,3-dicarboxamide

Measured: -2.06

Predicted: -2.20

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lomeprol

Measured: -2.79

Predicted: -2.72