

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.21e-12 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.34e-01

Confidence level: 3.54e-01

Nearest Neighbors from the Training Set

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Cloxyfonac [ISO]

Measured: 6.86e-12

Predicted: 3.84e-07

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4-Chloro-3-methylphenol

Measured: 1.50e-12

Predicted: 5.35e-02

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2,4,6-Trimethylpyridine

Measured: 3.59e-10

Predicted: 8.58e-01

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2,2,5,5-Tetramethylhexane

Measured: 9.80e-08

Predicted: 7.94

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1-Isobutoxypropan-2-ol

Measured: 7.13e-08

Predicted: 1.69