

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.08 days

Global applicability domain: Outside

Local applicability domain index: 9.18e-02

Confidence level: 8.19e-01

Nearest Neighbors from the Training Set

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Pentane

Measured: 40.7

Predicted: 6.52

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2-Methylheptane

Measured: 12.5

Predicted: 3.99

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2-Methylhexane

Measured: 12.5

Predicted: 5.54

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2-Methyloctane

Measured: 40.7

Predicted: 4.23

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3-Methyloctane

Measured: 40.7

Predicted: 4.08