

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.18×10^{-11} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.20×10^{-1}

Confidence level: 6.65×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Triethyl phosphate

Measured: 5.53×10^{-11}

Predicted: 4.26×10^{-11}

Image not found

Diethyl sulfate

Measured: 1.80×10^{-12}

Predicted: 1.55×10^{-12}

Image not found

Phosphoramidic acid, dimethyl-, dimethyl ester

Measured: 3.19×10^{-11}

Predicted: 2.75×10^{-11}

Image not found

Propylene dinitrate

Measured: 3.20×10^{-13}

Predicted: 3.59×10^{-13}

Image not found

O,O-Dimethyl phosphoramidothioate

Measured: 2.44×10^{-10}

Predicted: 1.11×10^{-10}