

Trimethyl phosphate
512-56-1 | DTXSID1021403

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: 1.67e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.29e-01

Confidence level: 6.16e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Trimethyl phosphate

Measured: 7.37e-12

Predicted: 1.67e-11

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O,O-Dimethyl
chlorothiophosphate

Measured: 5.90e-11

Predicted: 4.05e-11

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O,O,O-Trimethyl
phosphorothioate

Measured: 6.97e-11

Predicted: 4.29e-11

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O,O,S-Trimethyl
phosphorothioate

Measured: 9.29e-12

Predicted: 1.56e-11

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O,O-Dimethyl
phosphoramidothioate

Measured: 2.44e-10

Predicted: 1.11e-10