

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.50

Global applicability domain: Inside

Local applicability domain index: 4.74e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

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Trimethyl phosphate

Measured: 1.41

Predicted: 1.50

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Cyanoguanidine

Measured: 3.09

Predicted: 2.93

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Triethyl phosphate

Measured: 1.29

Predicted: 1.38

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1,1'-Oxybis-2-propanol

Measured: 4.57

Predicted: 3.83

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Hexamethylphosphoramide

Measured: 5.01e-01

Predicted: 7.23e-01