

Triethyl phosphate
78-40-0 | DTXSID8026228

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 8.20e-01

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

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Triethyl phosphate

Measured: 0.8

Predicted: 8.20e-01

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Phosphonic acid, bis(1-methylethyl) ester

Measured: 0.45

Predicted: 5.25e-01

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Diisopropyl fluorophosphate

Measured: 1.17

Predicted: 1.28

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Tripropyl phosphate

Measured: 1.87

Predicted: 1.92

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cis-Mevinphos

Measured: 0.13

Predicted: 9.28e-02