

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -54.1 °C

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

Image not found

Triethyl phosphate

Measured: -56.4

Predicted: -54.1

Image not found

Trimethyl phosphate

Measured: -46.0

Predicted: -49.9

Image not found

Tributyl phosphate

Measured: -79.0

Predicted: -70.4

Image not found

Dimethyl hydrogen phosphite

Measured: -60.0

Predicted: -61.6