

O,O-Diethyl dithiophosphate
298-06-6 | DTXSID6027133

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 9.37 days

Global applicability domain: Outside

Local applicability domain index: 1.69e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

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9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A

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Benzothiophene

Measured: 1650

Predicted: 21.4

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5-Methylindan

Measured: 4.93

Predicted: 2.25

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2-Methylphenanthrene

Measured: 1370

Predicted: 25.0

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4-Methylindan

Measured: 4.93

Predicted: 2.31