

Diisopropyl fluorophosphate
55-91-4 | DTXSID1040667

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: 4.91 days

Global applicability domain: Outside

Local applicability domain index: 8.16e-02

Confidence level: 8.23e-01

Nearest Neighbors from the Training Set

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Pentane

Measured: 40.7

Predicted: 6.52

[Image not found](#)

n-Hexane

Measured: 157

Predicted: 7.45

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2-Methylhexane

Measured: 12.5

Predicted: 5.54

[Image not found](#)

Heptane

Measured: 88.3

Predicted: 7.54

[Image not found](#)

2-Methylheptane

Measured: 12.5

Predicted: 3.99