

Phosphonothioic acid, methyl-, O,o-diethyl ester
6996-81-2 | DTXSID10220237

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: 10.4

Global applicability domain: Inside

Local applicability domain index: 5.19e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

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O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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Dioxabenzofos

Measured: 20.4

Predicted: 13.7

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Methyl parathion

Measured: 85.1

Predicted: 14.5

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Menthol

Measured: 10.8

Predicted: 23.5

[Image not found](#)

(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5

[Image not found](#)

Isophorone

Measured: 2.00

Predicted: 3.19