

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

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

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: 4.44 days

Global applicability domain: Outside

Local applicability domain index: 2.97e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

[Image not found](#)

5-Methylindan

Measured: 4.93

Predicted: 2.25

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Propylbenzene

Measured: 24.3

Predicted: 4.02

[Image not found](#)

Ethylbenzene

Measured: 120

Predicted: 6.21

[Image not found](#)

4-Ethyltoluene

Measured: 24.3

Predicted: 3.95

[Image not found](#)

1,3-Diethylbenzene

Measured: 88.3

Predicted: 5.36