

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 |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

Model Results

Predicted value: 3.71e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.37e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

Image not found

Triethyl phosphate

Measured: 5.53e-11

Predicted: 4.26e-11

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Phosphoramidic acid, dimethyl-,
dimethyl ester

Measured: 3.19e-11

Predicted: 2.75e-11

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Dimefox

Measured: 6.40e-11

Predicted: 3.64e-11

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O,S,S-Trimethyl
phosphorodithioate

Measured: 9.59e-12

Predicted: 1.50e-11

Image not found

O,O,S- Trimethyl dithiophosphate

Measured: 5.60e-11

Predicted: 3.74e-11