

3H-1,2-Dithiole-3-thione, 4-methyl-
3354-41-4 | DTXSID30187196

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: 5.11e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.82e-01

Confidence level: 7.04e-01

Nearest Neighbors from the Training Set

Image not found

Ethylketene

Measured: 1.18e-10

Predicted: 9.07e-11

Image not found

Methylketene

Measured: 7.00e-11

Predicted: 6.39e-11

Image not found

(Z)-Dichloropropene

Measured: 1.12e-11

Predicted: 1.42e-11

Image not found

trans-1,3-Dichloropropene

Measured: 1.12e-11

Predicted: 1.42e-11

Image not found

1-Propen-1-one, 2-methyl-

Measured: 1.07e-10

Predicted: 9.66e-11

Image not found

3-Methylbutanal

Measured: 2.74e-11

Predicted: 2.76e-11