

Dimethyl sulfoxide
67-68-5 | DTXSID2021735

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: 1.83e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.65e-01

Confidence level: 5.13e-01

Nearest Neighbors from the Training Set

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Dimethyl sulfoxide

Measured: 6.20e-11

Predicted: 1.83e-11

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Acetaldehyde oxime

Measured: 2.20e-12

Predicted: 2.06e-12

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N-Nitrosodimethylamine

Measured: 2.53e-12

Predicted: 1.27e-12

Image not found

2-Nitropropane

Measured: 2.60e-13

Predicted: 3.96e-13

Image not found

1-Nitropropane

Measured: 4.40e-13

Predicted: 5.94e-13