

n-Hexane
110-54-3 | DTXSID0021917

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: 5.55e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.26e-01

Confidence level: 9.08e-01

Nearest Neighbors from the Training Set

Image not found

n-Hexane

Measured: 5.61e-12

Predicted: 5.55e-12

Image not found

2-Methylbutane

Measured: 3.90e-12

Predicted: 4.63e-12

Image not found

2,3-Dimethylbutane

Measured: 6.20e-12

Predicted: 4.81e-12

Image not found

Heptane

Measured: 7.15e-12

Predicted: 6.52e-12

Image not found

3-Methylpentane

Measured: 5.70e-12

Predicted: 5.37e-12