

1-Methylpyrene  
2381-21-7 | DTXSID0025654

### Model Performance

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

#### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87            | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

## Model Results

**Predicted value:** 7.51e-07 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 5.06e-01

**Confidence level:** 5.62e-01

## Nearest Neighbors from the Training Set

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Dienochlor

**Measured:** 5.27e-08

**Predicted:** 8.74e-08

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Mirex

**Measured:** 1.56e-07

**Predicted:** 1.49e-07

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Kepone

**Measured:** 5.50e-06

**Predicted:** 2.03e-06

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Naphthalene, 1-iodo-

**Measured:** 2.82e-05

**Predicted:** 1.16e-05

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Fluoranthene

**Measured:** 1.14e-06

**Predicted:** 1.33e-06