

2-Methylnaphthalene  
91-57-6 | DTXSID4020878

### 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:** 1.39e-05 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 6.40e-01

**Confidence level:** 5.50e-01

## Nearest Neighbors from the Training Set

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Octachlorocyclopentene

**Measured:** 2.91e-07

**Predicted:** 1.00e-06

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Hexachlorocyclopentadiene

**Measured:** 6.60e-06

**Predicted:** 9.10e-06

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Propane, 1,3-dibromo-2,2-bis(bromomethyl)-

**Measured:** 4.13e-06

**Predicted:** 7.44e-06

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Benzene, iodo-

**Measured:** 1.67e-03

**Predicted:** 5.90e-03

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Benzothiophene

**Measured:** 9.69e-04

**Predicted:** 6.71e-03