

Deacetylmoxisylyte  
35231-36-8 | DTXSID10188722

### 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:** 6.59e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 1.92e-01

**Confidence level:** 8.52e-01

## Nearest Neighbors from the Training Set

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alpha-Phellandrene

**Measured:** 3.13e-10

**Predicted:** 2.83e-10

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

**Measured:** 4.80e-11

**Predicted:** 4.73e-11

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alpha-Cedrene

**Measured:** 6.70e-11

**Predicted:** 7.41e-11

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(-)-alpha-Coen

**Measured:** 9.00e-11

**Predicted:** N/A

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Isoproturon

**Measured:** 1.20e-11

**Predicted:** 3.23e-11