

Tetradeca-1,13-diene  
21964-49-8 | DTXSID80176373

### Model Performance

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

#### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.84            | 0.55 | 0.85           | 0.53 | 0.83       | 0.64 |

## Model Results

**Predicted value:** 931

**Global applicability domain:** Inside

**Local applicability domain index:** 3.05e-01

**Confidence level:** 6.00e-01

## Nearest Neighbors from the Training Set

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Dibenz[a,h]acridine

**Measured:** 107

**Predicted:** 81.4

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Hexadecane

**Measured:** 5010

**Predicted:** 3680

Image not found

Fluoranthene

**Measured:** 3630

**Predicted:** 339

Image not found

Pyrene

**Measured:** 1510

**Predicted:** 344

Image not found

Benz(a)anthracene

**Measured:** 257

**Predicted:** 1240