

3H-1,2-Dithiole-3-thione, 4-methyl-  
3354-41-4 | DTXSID30187196

### Model Performance

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

#### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.72            | 51.8 | 0.74           | 50.3 | 0.73       | 52.7 |

## Model Results

**Predicted value:** 55.0 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 5.64e-01

**Confidence level:** 5.84e-01

## Nearest Neighbors from the Training Set

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1,3-Dithiolane-2-thione

**Measured:** 35.0

**Predicted:** 46.9

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Methanone, di-2-thienyl-

**Measured:** 90.0

**Predicted:** 49.4

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1,3-Dithiole-2-thione

**Measured:** 49.0

**Predicted:** 44.2

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alpha-Terthiophene

**Measured:** 93.5

**Predicted:** 69.2