

2,3,4-Trimethylpentane  
565-75-3 | DTXSID6060343

### 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:** -111 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 9.90e-01

**Confidence level:** 8.72e-01

## Nearest Neighbors from the Training Set

Image not found

2,3,4-Trimethylpentane

**Measured:** -109

**Predicted:** -111

Image not found

Pentane, 2,3,3-trimethyl-

**Measured:** -101

**Predicted:** -106

Image not found

(3S)-2,2,3-Trimethylpentane

**Measured:** -112

**Predicted:** -107

Image not found

2,2,4-Trimethylpentane

**Measured:** -107

**Predicted:** -106