

2-Methylhexane  
591-76-4 | DTXSID5052256

### Model Performance

Model	Data
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#### Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 89.5 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 1.00

**Confidence level:** 9.27e-01

## Nearest Neighbors from the Training Set

Image not found

3-Methylhexane

**Measured:** 91.0

**Predicted:** 89.5

Image not found

2-Methylhexane

**Measured:** 90.0

**Predicted:** 89.5

Image not found

Pentane, 3-ethyl-

**Measured:** 93.5

**Predicted:** 89.5

Image not found

Pentane,3,3-dimethyl-

**Measured:** 86.0

**Predicted:** 84.5

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Pentane, 2,2-dimethyl-

**Measured:** 79.2

**Predicted:** 84.5