

2-Methylheptane  
592-27-8 | DTXSID2060460

### 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
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 8.23e-06 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 8.44e-01

**Confidence level:** 6.61e-01

## Nearest Neighbors from the Training Set

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2,3,4-Trimethylpentane

**Measured:** 2.01e-05

**Predicted:** 1.15e-05

Image not found

Hexane, 2,2-dimethyl-

**Measured:** 1.75e-06

**Predicted:** 8.30e-06

Image not found

Octane

**Measured:** 5.78e-06

**Predicted:** 9.23e-06

Image not found

2,2,4-Trimethylpentane

**Measured:** 1.96e-05

**Predicted:** 1.08e-05