

1,3,5-Cycloheptatriene  
544-25-2 | DTXSID5073909

### 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
0.95	0.69	0.95	0.65	0.96	0.68

## Model Results

**Predicted value:** 3.89

**Global applicability domain:** Inside

**Local applicability domain index:** 9.91e-01

**Confidence level:** 5.64e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Dimethyl sulfoxide

**Measured:** 4.96

**Predicted:** 3.99

[Image not found](#)

Toluene

**Measured:** 3.31

**Predicted:** 3.87

[Image not found](#)

Hexanal

**Measured:** 4.41

**Predicted:** 3.86

[Image not found](#)

Methylcyclohexane

**Measured:** 3.03

**Predicted:** 3.59

[Image not found](#)

2-Hexanone

**Measured:** 3.68

**Predicted:** 3.66