

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

### 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:** -74.2 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 8.78e-01

**Confidence level:** 5.60e-01

## Nearest Neighbors from the Training Set

Image not found

1,3,5-Cycloheptatriene

**Measured:** -79.5

**Predicted:** -74.2

Image not found

1,3-Cyclopentadiene

**Measured:** -85.0

**Predicted:** -83.9

Image not found

1,3,5,7-Cyclooctatetraene

**Measured:** -4.70

**Predicted:** -37.8

Image not found

Cyclohepta-1,3-diene

**Measured:** -110

**Predicted:** -75.9