

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.23e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.18e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

Image not found

1,3,5-Cycloheptatriene

Measured: 6.73e-03

Predicted: 4.23e-03

Image not found

1,4-Dibromobutane

Measured: 1.62e-03

Predicted: 2.55e-03

Image not found

1,4-Cyclohexadiene

Measured: 8.74e-03

Predicted: 7.68e-03