

3-Methylhexane
589-34-4 | DTXSID3044334

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.10

Global applicability domain: Inside

Local applicability domain index: 6.18e-01

Confidence level: 7.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

3-Methylpentane

Measured: 3.60

Predicted: 3.59

[Image not found](#)

Heptane

Measured: 4.66

Predicted: 4.56

[Image not found](#)

Heptane, 1-chloro-

Measured: 4.15

Predicted: 4.21

[Image not found](#)

Methylcyclohexane

Measured: 3.61

Predicted: 3.74

[Image not found](#)

Ethylcyclohexane

Measured: 4.56

Predicted: 4.45