

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 89.5 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 9.27e-01

Nearest Neighbors from the Training Set

Image not found

3-Methylhexane

Measured: 91.0

Predicted: 89.5

Image not found

2-Methylhexane

Measured: 90.0

Predicted: 89.5

Image not found

Pentane, 3-ethyl-

Measured: 93.5

Predicted: 89.5

Image not found

Pentane,3,3-dimethyl-

Measured: 86.0

Predicted: 84.5

Image not found

Pentane, 2,2-dimethyl-

Measured: 79.2

Predicted: 84.5