

1-Hexene
592-41-6 | DTXSID4025402

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 66.1 °C

Global applicability domain: Inside

Local applicability domain index: 9.46e-01

Confidence level: 9.23e-01

Nearest Neighbors from the Training Set

Image not found

1-Hexene

Measured: 63.4

Predicted: 66.1

Image not found

2-Butene, 2,3-dimethyl-

Measured: 73.3

Predicted: 68.2

Image not found

3-Methylenepentane

Measured: 64.7

Predicted: 63.6

Image not found

2-Methylpent-1-ene

Measured: 62.1

Predicted: 93.3

Image not found

2-Pentene, 3-methyl-

Measured: 69.0

Predicted: 68.5