

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.35

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 7.53e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Hexene

Measured: 3.39

Predicted: 3.35

[Image not found](#)

1-Heptene

Measured: 3.99

Predicted: 3.99

[Image not found](#)

2,5-Dimethyl-2,4-hexadiene

Measured: 3.50

Predicted: 3.50

[Image not found](#)

Pentane

Measured: 3.39

Predicted: 3.15