

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 160 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.23e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

Image not found

n-Butyl chloroformate

Measured: 184

Predicted: 6.18

Image not found

1-Butene, 2,3-dimethyl-

Measured: 126

Predicted: 250

Image not found

1,5-Hexadiene

Measured: 165

Predicted: 208

Image not found

1,2,5,6,9,10-

Hexabromocyclododecane

Measured: 104

Predicted: 6.19e-07

Image not found

1,1-Dichloropropene

Measured: 252

Predicted: 66.1