

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.62×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.31×10^{-1}

Confidence level: 9.57×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1-Hexene

Measured: 3.75×10^{-11}

Predicted: 3.62×10^{-11}

Image not found

1-Heptene

Measured: 4.05×10^{-11}

Predicted: 3.79×10^{-11}

Image not found

1-Pentene

Measured: 3.19×10^{-11}

Predicted: 3.30×10^{-11}

Image not found

3-Methyl-1-butene

Measured: 3.18×10^{-11}

Predicted: 3.27×10^{-11}

Image not found

1-Butene

Measured: 3.14×10^{-11}

Predicted: 3.13×10^{-11}