

Nonene
27215-95-8 | DTXSID6027927

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: 4.98

Global applicability domain: Inside

Local applicability domain index: 6.90e-01

Confidence level: 7.53e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Nonene

Measured: 5.15

Predicted: 5.10

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(2E)-2-Octene

Measured: 4.51

Predicted: 4.48

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Octane

Measured: 5.18

Predicted: 5.05

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Cyclooctane

Measured: 4.45

Predicted: 4.49

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1-Decene

Measured: 5.70

Predicted: 5.54