

Myrcene
123-35-3 | DTXSID6025692

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.08e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.56e-01

Confidence level: 8.18e-01

Nearest Neighbors from the Training Set

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Myrcene

Measured: 4.11e-05

Predicted: 4.08e-05

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alpha-Pinene

Measured: 1.83e-05

Predicted: 3.40e-05

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gamma-Terpinene

Measured: 6.37e-05

Predicted: 4.78e-05

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Limonene

Measured: 7.77e-05

Predicted: 5.10e-05

[Image not found](#)

D-Limonene

Measured: 7.77e-05

Predicted: 5.10e-05

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Camphene

Measured: 3.38e-05

Predicted: 3.87e-05