

Myrcene
123-35-3 | DTXSID6025692

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -63.4 °C

Global applicability domain: Inside

Local applicability domain index: 8.99e-01

Confidence level: 3.06e-01

Nearest Neighbors from the Training Set

Image not found

(3Z)-1,3-Pentadiene

Measured: -114

Predicted: -82.5

Image not found

(3E)-1,3-Pentadiene

Measured: -114

Predicted: -82.5

Image not found

1,4-Hexadiene

Measured: -139

Predicted: -55.7

Image not found

1,3-Pentadiene, 2-methyl-

Measured: 75.5

Predicted: -72.9

Image not found

1,4-Pentadiene

Measured: -149

Predicted: -136