

beta-Ocimene
13877-91-3 | DTXSID70274135

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: 3.97 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.02e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Hydroquinone

Measured: 2.01

Predicted: 9.78e-05

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alpha-Bromotoluene

Measured: 15.7

Predicted: 4.50e-01

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2-Propanone, 1-chloro-1,1,3,3,3-pentafluoro-

Measured: 2.50

Predicted: 2670

[Image not found](#)

4-(2-Methylbutan-2-yl)phenol

Measured: 4.75

Predicted: 1.11e-02

[Image not found](#)

Dimethylamine

Measured: 2.93

Predicted: 664