

beta-Caryophyllene
87-44-5 | DTXSID8024739

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: 4.80e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.00e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

Image not found

2-Pyrrolicarboxylic acid

Measured: 2.00e-03

Predicted: 2.86e-05

Image not found

Carbophenothion

Measured: 3.99e-02

Predicted: 4.02e-07

Image not found

Naphthalene

Measured: 1.08e-01

Predicted: 2.15e-08

Image not found

Benzophenone

Measured: 3.68e-01

Predicted: 7.04e-04

Image not found

4'-Methoxyacetophenone

Measured: 2.46e-01

Predicted: 1.65e-02