

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1070

Global applicability domain: Inside

Local applicability domain index: 4.88e-01

Confidence level: 5.86e-01

Nearest Neighbors from the Training Set

Image not found

2,2,4,6,6-Pentamethylheptane

Measured: 871

Predicted: 963

Image not found

1,5,9-Cyclododecatriene

Measured: 8320

Predicted: 4560

Image not found

4-(1,1,3,3-Tetramethylbutyl)phenol

Measured: 288

Predicted: 134

Image not found

2,4-Di-tert-butylphenol

Measured: 251

Predicted: 202

Image not found

1,3-Diisopropylbenzene

Measured: 1910

Predicted: 374