

beta-Caryophyllene
87-44-5 | DTXSID8024739

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 2.55 days

Global applicability domain: Outside

Local applicability domain index: 3.46e-01

Confidence level: 8.92e-01

Nearest Neighbors from the Training Set

Image not found

4-Methylindan

Measured: 4.93

Predicted: 2.31

Image not found

3-Methylindene

Measured: 12.5

Predicted: 2.76

Image not found

1H-Indene, 2-methyl-

Measured: 12.5

Predicted: 2.48

Image not found

5-Methylindan

Measured: 4.93

Predicted: 2.25

Image not found

Indene

Measured: 12.5

Predicted: 7.90