

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.99e-10 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.61e-01

Confidence level: 9.06e-01

Nearest Neighbors from the Training Set

Image not found

beta-Caryophyllene

Measured: 2.00e-10

Predicted: 1.99e-10

Image not found

D-Limonene

Measured: 1.71e-10

Predicted: 1.73e-10

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Linalool

Measured: 1.60e-10

Predicted: 1.65e-10

Image not found

Myrcene

Measured: 2.15e-10

Predicted: 2.05e-10

Image not found

Ocimene (E)

Measured: 2.52e-10

Predicted: 2.40e-10

Image not found

beta-Ocimene

Measured: 2.52e-10

Predicted: 2.40e-10