

alpha-Humulene
6753-98-6 | DTXSID30858793

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: 2.87e-10 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.24e-01

Confidence level: 8.28e-01

Nearest Neighbors from the Training Set

Image not found

alpha-Humulene

Measured: 2.90e-10

Predicted: 2.87e-10

Image not found

alpha-Terpinene

Measured: 3.63e-10

Predicted: 2.91e-10

Image not found

gamma-Terpinene

Measured: 1.77e-10

Predicted: 2.06e-10

Image not found

Terpinolene

Measured: 2.25e-10

Predicted: 2.22e-10

Image not found

alpha-Phellandrene

Measured: 3.13e-10

Predicted: 2.83e-10