

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 5.73

Global applicability domain: Inside

Local applicability domain index: 4.70e-01

Confidence level: 5.91e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methyl tetradecanoate

Measured: 6.41

Predicted: 6.33

[Image not found](#)

Propyl laurate

Measured: 6.11

Predicted: 6.20

[Image not found](#)

Butyl laurate

Measured: 6.51

Predicted: 6.53

[Image not found](#)

1-Tetradecanol

Measured: 6.03

Predicted: 6.03