

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 250 °C

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 7.83e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Longifolene

Measured: 258

Predicted: 261

[Image not found](#)

1,2,4-Triisopropylbenzene

Measured: 244

Predicted: 250

[Image not found](#)

1,3,5-Triisopropylbenzene

Measured: 238

Predicted: 250

[Image not found](#)

Benzene, octyl-

Measured: 265

Predicted: 264