

alpha-Humulene
6753-98-6 | DTXSID30858793

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 1250

Global applicability domain: Inside

Local applicability domain index: 4.26e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

Image not found

2,2,4,6,6-Pentamethylheptane

Measured: 871

Predicted: 963

Image not found

1,5,9-Cyclododecatriene

Measured: 8320

Predicted: 4560

Image not found

4-(1,1,3,3-Tetramethylbutyl)phenol

Measured: 288

Predicted: 134

Image not found

2,4-Di-tert-butylphenol

Measured: 251

Predicted: 202

Image not found

2,2,4,4,6,8,8-Heptamethylnonane

Measured: 6610

Predicted: 6010