

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 |
| 0.95 | 0.69 | 0.95 | 0.65 | 0.96 | 0.68 |

Model Results

Predicted value: 6.90

Global applicability domain: Inside

Local applicability domain index: 9.88e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

[Image not found](#)

trans-Stilbene

Measured: 7.48

Predicted: 6.90

[Image not found](#)

1,2-Dichloronaphthalene

Measured: 6.89

Predicted: 6.90

[Image not found](#)

1,5-Dichloronaphthalene

Measured: 6.65

Predicted: 6.90

[Image not found](#)

1,4-Dichloronaphthalene

Measured: 6.78

Predicted: 6.90

[Image not found](#)

2,7-Dichloronaphthalene

Measured: 6.70

Predicted: 6.90