

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
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 7500 L/kg

**Global applicability domain:** Outside

**Local applicability domain index:** 3.68e-01

**Confidence level:** 8.11e-01

## Nearest Neighbors from the Training Set

Image not found

2,2'-Dichlorobiphenyl

**Measured:** 8320

**Predicted:** 13100

Image not found

2,4'-Dichlorobiphenyl

**Measured:** 21900

**Predicted:** 21900

Image not found

2,2',5-Trichlorobiphenyl

**Measured:** 25100

**Predicted:** 35900

Image not found

2-Chlorobiphenyl

**Measured:** 2950

**Predicted:** 3250

Image not found

4'-Acetylbiphenyl

**Measured:** 1660

**Predicted:** 1580