

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.52e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 7.99e-01

Nearest Neighbors from the Training Set

Image not found

tert-Pentylbenzene

Measured: 7.08e-05

Predicted: 3.93e-05

Image not found

Benzene, hexyl-

Measured: 5.56e-06

Predicted: 6.88e-06

Image not found

p-Menthane

Measured: 2.00e-06

Predicted: 2.12e-06

Image not found

Heptylbenzene

Measured: 2.54e-06

Predicted: 3.24e-06

Image not found

Cyclopentane, pentyl-

Measured: 8.20e-07

Predicted: 1.76e-06