

propan-2-yl naphthalen-1-ylacetate
68360-82-7 | DTXSID60286262

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: 2.37e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 4.22e-01

Nearest Neighbors from the Training Set

Image not found

Oxabentrinil

Measured: 8.61e-05

Predicted: 1.53e-03

Image not found

alpha-Santonin

Measured: 8.12e-04

Predicted: 5.45e-04

Image not found

Siduron

Measured: 7.75e-05

Predicted: 2.20e-03

Image not found

Benquinox

Measured: 2.07e-05

Predicted: 3.02e-02