

Ethyl 1-naphthaleneacetate
2122-70-5 | DTXSID3034583

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 313 °C

Global applicability domain: Inside

Local applicability domain index: 6.24e-01

Confidence level: 8.49e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl 2-naphthoate

Measured: 309

Predicted: 307

Image not found

Ethyl 1-naphthoate

Measured: 310

Predicted: 307

Image not found

1-(2-Naphthyl)propan-1-one

Measured: 313

Predicted: 306

Image not found

3-Ethoxy-1,1'-biphenyl

Measured: 305

Predicted: 294