

6-Methylsalicylic acid
567-61-3 | DTXSID20205257

Model Performance

Model	Data
-------	------

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: 263 °C

Global applicability domain: Inside

Local applicability domain index: 2.57e-01

Confidence level: 4.86e-01

Nearest Neighbors from the Training Set

Image not found

2-Hydroxyphenylacetic acid

Measured: 240

Predicted: 261

Image not found

Benzoic acid, 2,6-dimethyl-

Measured: 275

Predicted: 270

Image not found

Benzoic acid, 2,4-dimethyl-

Measured: 268

Predicted: 270