

D-(-)-Mandelic acid
611-71-2 | DTXSID4046523

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: 263 °C

Global applicability domain: Inside

Local applicability domain index: 2.59e-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

2-Chlorobenzoic acid

Measured: 287

Predicted: 273

Image not found

Benzoic acid, 2,6-dimethyl-

Measured: 275

Predicted: 270

Image not found

Benzoic acid, 2,4-dimethyl-

Measured: 268

Predicted: 270