

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 132 °C

Global applicability domain: Inside

Local applicability domain index: 7.73e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

Image not found

Mandelic acid

Measured: 124

Predicted: 132

Image not found

Mandelic acid

Measured: 124

Predicted: 132

Image not found

Mandelic acid

Measured: 124

Predicted: 132

Image not found

Mandelic acid

Measured: 124

Predicted: 132

Image not found

2-Hydroxyphenylacetic acid

Measured: 148

Predicted: 140

Image not found

3-Hydroxyphenylacetic acid

Measured: 132

Predicted: 147

Image not found

Benzenepropanoic acid, 4-hydroxy-

Measured: 131

Predicted: 135

Image not found

Benzeneacetic acid, 4-hydroxy-

Measured: 152

Predicted: 160

