

Salicylic acid
69-72-7 | DTXSID7026368

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: 162 °C

Global applicability domain: Inside

Local applicability domain index: 8.14e-01

Confidence level: 7.93e-01

Nearest Neighbors from the Training Set

Image not found

Salicylic acid

Measured: 158

Predicted: 162

Image not found

5-Methylsalicylic acid

Measured: 151

Predicted: 164

Image not found

m-Cresotic acid

Measured: 177

Predicted: 167

Image not found

6-Methylsalicylic acid

Measured: 173

Predicted: 167

Image not found

2-Hydroxy-3-methylbenzoic acid

Measured: 166

Predicted: 166