

Benzoic acid, 2-methoxy-
579-75-9 | DTXSID3060376

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: 130 °C

Global applicability domain: Inside

Local applicability domain index: 9.42e-01

Confidence level: 4.47e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 2-methoxy-

Measured: 101

Predicted: 130

Image not found

Benzoic acid, 3-methoxy-

Measured: 107

Predicted: 133

Image not found

Benzoic acid, 4-methoxy-

Measured: 185

Predicted: 139

Image not found

Benzeneacetic acid, 4-methoxy-

Measured: 87.0

Predicted: 121

Image not found

Benzoic acid, 4-ethoxy-

Measured: 198

Predicted: 128