

Benzoic acid, 3-methoxy-
586-38-9 | DTXSID2060410

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.18

Global applicability domain: Inside

Local applicability domain index: 7.01e-01

Confidence level: 6.71e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl salicylate

Measured: 2.95

Predicted: 2.38

Image not found

Benzoic acid, 3-methoxy-

Measured: 2.02

Predicted: 2.18

Image not found

3-Methoxyphenylacetic acid

Measured: 1.50

Predicted: 2.04

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Benzoic acid, 4-methoxy-

Measured: 1.96

Predicted: 2.18

Image not found

Ethylparaben

Measured: 2.47

Predicted: 2.13