

4-Hydroxy-3-methoxybenzaldehyde
121-33-5 | DTXSID0021969

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: 94.6 °C

Global applicability domain: Inside

Local applicability domain index: 8.57e-01

Confidence level: 6.83e-01

Nearest Neighbors from the Training Set

Image not found

4-Hydroxy-3-methoxybenzaldehyde

Measured: 81.5

Predicted: 94.6

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3-Hydroxy-4-methoxybenzaldehyde

Measured: 114

Predicted: 97.7

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Acetovanillone

Measured: 115

Predicted: 97.9

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3-Ethoxy-4-hydroxybenzaldehyde

Measured: 77.5

Predicted: 92.7

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4-Hydroxy-3-methoxycinnamaldehyde

Measured: 84.0

Predicted: 99.0