

Methylparaben

99-76-3 | DTXSID4022529

Model Performance

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: 98.7 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

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Methylparaben

Measured: 131

Predicted: 98.7

[Image not found](#)

Methyl 3-hydroxybenzoate

Measured: 73.0

Predicted: 95.8

[Image not found](#)

Ethylparaben

Measured: 117

Predicted: 101

[Image not found](#)

Ethyl 3-hydroxybenzoate

Measured: 74.0

Predicted: 93.5