

Methylparaben

99-76-3 | DTXSID4022529

Model Performance

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1.49

Global applicability domain: Inside

Local applicability domain index: 7.11e-01

Confidence level: 7.51e-01

Nearest Neighbors from the Training Set

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Urea, 1-(p-fluorophenyl)-

Measured: 1.52

Predicted: 1.70

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 1.29

Predicted: 1.47

[Image not found](#)

(2-Fluorophenyl)urea

Measured: 1.32

Predicted: 1.72

[Image not found](#)

Urea, (m-fluorophenyl)-

Measured: 1.77

Predicted: 1.77

[Image not found](#)

Urea, (3-methylphenyl)-

Measured: 1.56

Predicted: 1.57