

Ethyl 3-hydroxybenzoate
7781-98-8 | DTXSID10228435

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 65.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.05e-01

Confidence level: 8.31e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-(3-chlorophenyl)-N'-methylurea

Measured: 85.1

Predicted: 101

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

[Image not found](#)

Methyl N-(3-chlorophenyl)carbamate

Measured: 141

Predicted: 94.1

[Image not found](#)

[3-(Trifluoromethyl)phenyl]urea

Measured: 95.5

Predicted: 94.0