

Ethanone, 1-(2,4-dihydroxyphenyl)-
89-84-9 | DTXSID4058998

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: 39.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.43e-01

Confidence level: 7.29e-01

Nearest Neighbors from the Training Set

Image not found

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2

Image not found

(2-Fluorophenyl)urea

Measured: 20.9

Predicted: 52.8

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Urea, (m-fluorophenyl)-

Measured: 58.9

Predicted: 59.1

Image not found

3-Chlorophenylurea

Measured: 102

Predicted: 57.3

Image not found

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8