

2,3-Dihydroxynaphthalene
92-44-4 | DTXSID2043903

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: 87.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

Image not found

1-Hydroxymethylnaphthalene

Measured: 148

Predicted: 406

Image not found

Acetamide, N-(3-(trifluoromethyl)phenyl)- (9CI)

Measured: 56.2

Predicted: 73.5

Image not found

1-Naphthaleneacetic acid

Measured: 158

Predicted: 165

Image not found

Acetamide, N-(3-nitrophenyl)-

Measured: 87.1

Predicted: 89.4

Image not found

Acetamide, N-(2-chlorophenyl)-

Measured: 38.0

Predicted: 49.2