

5-Methylsalicylic acid
89-56-5 | DTXSID20237472

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: 44.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.60e-01

Confidence level: 7.45e-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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(2-Chlorophenyl)urea

Measured: 40.7

Predicted: 51.3

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3-Chlorophenylurea

Measured: 102

Predicted: 57.3

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Urea, (m-fluorophenyl)-

Measured: 58.9

Predicted: 59.1