

Dimethylglyoxime
95-45-4 | DTXSID2044393

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: 58.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.74e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found

Anisole

Measured: 34.7

Predicted: 69.5

Image not found

p-Cresol

Measured: 501

Predicted: 95.9

Image not found

Resorcinol

Measured: 9.55

Predicted: 28.3

Image not found

2-Methoxyphenol

Measured: 36.3

Predicted: 41.2

Image not found

Toluene

Measured: 117

Predicted: 87.4