

4,4'-Methylenedianiline
101-77-9 | DTXSID6022422

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: 87.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.68e-01

Confidence level: 9.15e-01

Nearest Neighbors from the Training Set

Image not found

4,4'-Methylenedianiline

Measured: 97.7

Predicted: 87.8

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4,4'-Thiodianiline

Measured: 110

Predicted: 116

Image not found

N-(1,1-dimethyl-2-propynyl)-4-methoxybenzamide

Measured: 67.6

Predicted: 72.5

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Methylpropyzamide

Measured: 57.5

Predicted: 71.4

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4-Chloro-N-(1,1-dimethyl-2-propynyl)benzamide

Measured: 79.4

Predicted: 71.4