

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.58

Global applicability domain: Inside

Local applicability domain index: 5.33e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,8-Naphthalenediamine

Measured: 1.78

Predicted: 1.49

[Image not found](#)

2,3-Naphthalenediamine

Measured: 1.54

Predicted: 1.49

[Image not found](#)

1,5-Naphthalenediamine

Measured: 0.89

Predicted: 1.24

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4,4'-Methylenedianiline

Measured: 1.59

Predicted: 1.58

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4,4'-Thiodianiline

Measured: 2.18

Predicted: 1.78