

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.95e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.46e-01

Confidence level: 6.79e-01

Nearest Neighbors from the Training Set

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1,5-Naphthalenediamine

Measured: 2.40e-03

Predicted: 6.55e-03

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1,10-Phenanthroline

Measured: 1.49e-02

Predicted: 5.60e-03

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Eryptamine

Measured: 2.71e-03

Predicted: 5.31e-02

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1,8-Naphthalenediamine

Measured: 5.37e-03

Predicted: 5.83e-03

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1-Phenyl-2-thiourea

Measured: 1.62e-02

Predicted: 7.48e-02