

4,4'-Diaminostilbene
621-96-5 | DTXSID2022412

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: 1.44

Global applicability domain: Inside

Local applicability domain index: 5.67e-01

Confidence level: 7.44e-01

Nearest Neighbors from the Training Set

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2,2'-Biphenyldiamine

Measured: 1.34

Predicted: 1.33

Image not found

Benzidine

Measured: 1.34

Predicted: 1.32

Image not found

1,5-Naphthalenediamine

Measured: 0.89

Predicted: 1.24

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3,3'-Dimethylbenzidine

Measured: 2.34

Predicted: 1.51

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1-(1-Naphthyl)-2-thiourea

Measured: 1.65

Predicted: 1.87