

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 12.1

Global applicability domain: Inside

Local applicability domain index: 4.28e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

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Menthol

Measured: 10.8

Predicted: 23.5

[Image not found](#)

(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5

[Image not found](#)

Phenacetin

Measured: 30.2

Predicted: 3.76

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Oxydisulfoton

Measured: 1.00

Predicted: 1.63

[Image not found](#)

O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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Isoamyl ether

Measured: 170

Predicted: 137