

4,4'-Thiodianiline
139-65-1 | DTXSID9021344

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.66e-08 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.03e-01

Confidence level: 3.48e-01

Nearest Neighbors from the Training Set

Image not found

2-Phenylcyclohexanol

Measured: 2.69e-06

Predicted: 1.03e-02

Image not found

Fenuron

Measured: 1.21e-05

Predicted: 1.82e-05

Image not found

Butylated hydroxytoluene

Measured: 2.00e-10

Predicted: 3.94e-03

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Naphthalene, 1,2,4,7-tetrachloro-

Measured: 3.45e-10

Predicted: 1.23e-05

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Acetic acid, 2,2-dichloro-, methyl ester

Measured: 3.00e-09

Predicted: 11.5