

3H-1,2-Dithiole-3-thione, 4-methyl-
3354-41-4 | DTXSID30187196

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: 7.58e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.35e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

Image not found

Benzothiazole

Measured: 3.18e-02

Predicted: 2.15e-02

Image not found

Ethane, 1,2-diiodo-

Measured: 6.06e-04

Predicted: 1.27e-03

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Methylene iodide

Measured: 4.63e-03

Predicted: 2.75e-03

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N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 1.34e-02

Predicted: 1.36e-02

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1,4-Dithiane

Measured: 2.50e-02

Predicted: 1.47e-02