

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.20

Global applicability domain: Outside

Local applicability domain index: 4.22e-01

Confidence level: 5.53e-01

Nearest Neighbors from the Training Set

Image not found

3H-1,2-Dithiole-3-thione, 4-methyl-

Measured: 2.18

Predicted: 2.20

Image not found

Trichloroacetonitrile

Measured: 2.09

Predicted: 2.02

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2,3-Dibromothiophene

Measured: 3.53

Predicted: 3.53

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3H-1,2-Dithiol-3-one

Measured: 0.82

Predicted: 1.12