

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.26e-02 mmHg

Global applicability domain: Outside

Local applicability domain index: 4.01e-01

Confidence level: 3.62e-01

Nearest Neighbors from the Training Set

Image not found

Amitraz

Measured: 5.00e-02

Predicted: 1.07e-06

Image not found

Ethyl benzoate

Measured: 2.20e-03

Predicted: 1.61e-01

Image not found

2-Chloroacetophenone

Measured: 2.80e-06

Predicted: 4.94e-02

Image not found

1,3-Propanediol

Measured: 8.00e-01

Predicted: 4.31e-02

Image not found

3-Ethylpyridine

Measured: 5.61

Predicted: 5.67e-01