

Thiophene
110-02-1 | DTXSID8026145

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: 32.5 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.68e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

Image not found

Furan

Measured: 79.7

Predicted: 192

Image not found

3-Hydroxypropanenitrile

Measured: 18.4

Predicted: 1.16e-01

Image not found

Formic acid, vinyl ester

Measured: 3.40

Predicted: 207

Image not found

1-iodohexadecane

Measured: 24.9

Predicted: 1.85e-05