

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -56.2 °C

Global applicability domain: Inside

Local applicability domain index: 7.18e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Thiophene

Measured: -39.4

Predicted: -56.2

[Image not found](#)

Thiophene, 2-methyl-

Measured: -63.4

Predicted: -66.5

[Image not found](#)

Thiophene, 3-methyl-

Measured: -69.0

Predicted: -66.5

[Image not found](#)

3-Ethylthiophene

Measured: -89.1

Predicted: -62.3

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2,5-Dimethylthiophene

Measured: -62.6

Predicted: -61.7