

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 96.2 °C

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 8.33e-01

Nearest Neighbors from the Training Set

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Thiophene

Measured: 84.0

Predicted: 96.2

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Divinyl sulfide

Measured: 84.0

Predicted: 89.4

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2,3-Dichloro-1,3-butadiene

Measured: 98.0

Predicted: 99.1

[Image not found](#)

Thiophene, 2,3-dihydro-

Measured: 112

Predicted: 112

[Image not found](#)

Thiophene, 2-methyl-

Measured: 113

Predicted: 105