

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.27

Global applicability domain: Inside

Local applicability domain index: 9.98e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl propionate

Measured: 3.15

Predicted: 3.27

Image not found

Propyl acetate

Measured: 3.17

Predicted: 3.27

Image not found

N-Methylpyrrolidine

Measured: 3.64

Predicted: 3.27

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1,4-Dioxane

Measured: 3.18

Predicted: 3.27

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3-Pentanone

Measured: 3.20

Predicted: 3.27