

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 45.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.28e-01

Confidence level: 8.63e-01

Nearest Neighbors from the Training Set

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1,1-Dichloroethane

Measured: 30.2

Predicted: 34.4

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1,2-Dichloropropane

Measured: 46.8

Predicted: 48.0

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1,2-Dichloroethane

Measured: 33.1

Predicted: 32.5

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1,3-Dichloropropene

Measured: 46.2

Predicted: 49.4

[Image not found](#)

trans-1,3-Dichloropropene

Measured: 46.2

Predicted: 49.4

[Image not found](#)

Chlorobenzene

Measured: 141

Predicted: 106