

2,3-Dibromothiophene
3140-93-0 | DTXSID80185324

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 10.6 days

Global applicability domain: Outside

Local applicability domain index: 3.18e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

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Indan

Measured: 61.9

Predicted: 8.13

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Acenaphthylene

Measured: 4340

Predicted: 36.6

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Indene

Measured: 12.5

Predicted: 7.90

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Benzothiophene

Measured: 1650

Predicted: 21.4

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Tetralin

Measured: 120

Predicted: 12.2