

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.26e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.04e-01

Confidence level: 7.07e-01

Nearest Neighbors from the Training Set

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(Z)-1,2-Dichloroethylene

Measured: 2.48e-12

Predicted: 2.80e-12

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(E)-1,2-Dichloroethylene

Measured: 2.48e-12

Predicted: 2.80e-12

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Ethylketene

Measured: 1.18e-10

Predicted: 9.07e-11

[Image not found](#)

Methylketene

Measured: 7.00e-11

Predicted: 6.39e-11

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(Z)-Dichloropropene

Measured: 1.12e-11

Predicted: 1.42e-11

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trans-1,3-Dichloropropene

Measured: 1.12e-11

Predicted: 1.42e-11

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Furfural

Measured: 3.51e-11

Predicted: 5.73e-11

