

Tetrachloroethylene-13C1
287399-46-6 | DTXSID30481626

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.35

Global applicability domain: Outside

Local applicability domain index: 3.97e-01

Confidence level: 6.07e-01

Nearest Neighbors from the Training Set

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Tetrachloroethylene

Measured: 3.40

Predicted: 3.35

[Image not found](#)

2,3-Dibromothiophene

Measured: 3.53

Predicted: 3.53

[Image not found](#)

Hexachloro-1,3-butadiene

Measured: 4.78

Predicted: 4.65

[Image not found](#)

3H-1,2-Dithiole-3-thione, 4-methyl-

Measured: 2.18

Predicted: 2.20

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1,2-Dibromoethylene

Measured: 1.76

Predicted: 1.90