

Hexachloro-1,3-butadiene
87-68-3 | DTXSID7020683

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: 5.68 days

Global applicability domain: Outside

Local applicability domain index: 4.22e-01

Confidence level: 6.52e-01

Nearest Neighbors from the Training Set

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1,1-Dimethylcyclopentane

Measured: 880

Predicted: 10.9

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1,2,4,5-Tetramethylbenzene

Measured: 88.3

Predicted: 5.46

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1,2,3,4-Tetramethylbenzene

Measured: 24.3

Predicted: 3.95

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Naphthalene

Measured: 12.5

Predicted: 8.13

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1,2,3,5-Tetramethylbenzene

Measured: 12.5

Predicted: 3.31