

Diphenylamine
122-39-4 | DTXSID4021975

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: 6.47 days

Global applicability domain: Inside

Local applicability domain index: 5.24e-01

Confidence level: 6.71e-01

Nearest Neighbors from the Training Set

Image not found

Biphenyl

Measured: 2720

Predicted: 17.6

Image not found

Naphthalene

Measured: 12.5

Predicted: 8.13

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1,2,3,4-Tetramethylbenzene

Measured: 24.3

Predicted: 3.95

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1,2,4,5-Tetramethylbenzene

Measured: 88.3

Predicted: 5.46

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1,2,3,5-Tetramethylbenzene

Measured: 12.5

Predicted: 3.31