

Furan

110-00-9 | DTXSID6020646

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 43.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.46e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

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Measured: 31.5

Predicted: 43.4

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1,3-Cyclopentadiene

Measured: 41.0

Predicted: 54.4

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Ethene, 1,1'-oxybis-

Measured: 28.3

Predicted: 43.0

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1,2-Epoxy-3-butene

Measured: 68.0

Predicted: 59.2

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Furan, 2,3-dihydro-

Measured: 54.5

Predicted: 62.7