

Furan

110-00-9 | DTXSID6020646

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -89.3 °C

Global applicability domain: Inside

Local applicability domain index: 7.46e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

Image not found

Furan

Measured: -85.6

Predicted: -89.3

Image not found

2-Methylfuran

Measured: -87.5

Predicted: -88.1

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Methyl iodide

Measured: -66.4

Predicted: -98.6

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Furan, 2-ethenyl-

Measured: -94.0

Predicted: -86.8

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Allyl bromide

Measured: -119

Predicted: -115