

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.65

Global applicability domain: Inside

Local applicability domain index: 5.56e-01

Confidence level: 8.45e-01

Nearest Neighbors from the Training Set

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Furan

Measured: 1.34

Predicted: 1.65

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2-Methylfuran

Measured: 1.85

Predicted: 1.97

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1,3-Butadiene

Measured: 1.99

Predicted: 1.88

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(3Z)-1,3-Pentadiene

Measured: 2.40

Predicted: 2.48

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(3E)-1,3-Pentadiene

Measured: 2.40

Predicted: 2.48

[Image not found](#)

Chloromethane

Measured: 0.91

Predicted: 9.71e-01