

2,5-Furandione
108-31-6 | DTXSID7024166

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.08e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 5.11e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Succinic anhydride

Measured: 2.50e-01

Predicted: 2.69e-03

[Image not found](#)

Isopropyl chloroformate

Measured: 1.50e-03

Predicted: 17.3

[Image not found](#)

1,3-Dibromobenzene

Measured: 3.00e-03

Predicted: 2.38e-01

[Image not found](#)

2-Methyltetrahydrofuran

Measured: 9.80e-03

Predicted: 101