

Isobutyric anhydride
97-72-3 | DTXSID7026609

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: 7.93e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.11e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

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Benzoic acid, 2,3-dimethoxy-

Measured: 4.40e-01

Predicted: 6.89e-06

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2,4-Pentanedione

Measured: 1.36

Predicted: 3.07

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3-Mercaptopropanoic acid

Measured: 5.10

Predicted: 5.30e-02

[Image not found](#)

1,3-Diethylbenzene

Measured: 7.80e-01

Predicted: 9.75e-01

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Phenacetin

Measured: 2.06e-01

Predicted: 3.33e-06