

Butanoic anhydride
106-31-0 | DTXSID8026729

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.26

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23

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Acetamide, N-methyl-N-phenyl-

Measured: 1.51

Predicted: 2.53

[Image not found](#)

Molinate

Measured: 25.7

Predicted: 14.8

[Image not found](#)

Bromacil

Measured: 3.24

Predicted: 2.87

[Image not found](#)

4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69