

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 194 °C

Global applicability domain: Inside

Local applicability domain index: 7.41e-01

Confidence level: 7.95e-01

Nearest Neighbors from the Training Set

Image not found

Butanoic anhydride

Measured: 200

Predicted: 194

Image not found

Isobutyric anhydride

Measured: 183

Predicted: 185

Image not found

2-Butoxyethyl acetate

Measured: 192

Predicted: 191

Image not found

Ethyl 2,2-dimethylacetoacetate

Measured: 182

Predicted: 190

Image not found

Diisopropyl oxalate

Measured: 191

Predicted: 201