

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 185 °C

Global applicability domain: Inside

Local applicability domain index: 7.02e-01

Confidence level: 8.85e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isobutyric anhydride

Measured: 183

Predicted: 185

[Image not found](#)

Butanoic anhydride

Measured: 200

Predicted: 194

[Image not found](#)

2-Ethoxyethyl acrylate

Measured: 174

Predicted: 175

[Image not found](#)

2-Butoxyethyl acetate

Measured: 192

Predicted: 191