

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -56.2 °C

Global applicability domain: Inside

Local applicability domain index: 8.13e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isobutyric anhydride

Measured: -53.5

Predicted: -56.2

[Image not found](#)

Butanoic anhydride

Measured: -75.0

Predicted: -61.1

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Propanoic anhydride

Measured: -45.0

Predicted: -53.2