

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 54.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.85e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl hexanoate

Measured: 115

Predicted: 110

[Image not found](#)

2-Phenylethyl acetate

Measured: 77.6

Predicted: 98.8

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

[Image not found](#)

Ethyl phenylacetate

Measured: 77.6

Predicted: 103

[Image not found](#)

Aldicarb

Measured: 31.6

Predicted: 38.0