

Tetrahydrophthalic anhydride
85-43-8 | DTXSID3026516

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.237

Global applicability domain: Inside

Local applicability domain index: 4.80e-01

Confidence level: 4.40e-01

Nearest Neighbors from the Training Set

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AC1LCSQ4

Measured: 0.57

Predicted: 7.92e-01

[Image not found](#)

4-Hydroxy-3,5,6-trimethyl-2H-pyran-2-one

Measured: 0.36

Predicted: 4.33e-01

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Citolone

Measured: -0.350

Predicted: -0.591