

Quinic acid
86-68-0 | DTXSID70323339

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: 1.52

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

Image not found

2-Cyanophenyl acetate

Measured: 1.33

Predicted: 1.37

Image not found

Methyl 2-(acetylamino)benzoate

Measured: 1.65

Predicted: 1.25

Image not found

Acetanilide, 2'-acetyl-

Measured: 1.50

Predicted: 1.65

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Acetamide, N-(2-chlorophenyl)-

Measured: 1.28

Predicted: 1.62

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Benzoic acid, 2-
((acetylmethyl)amino)-

Measured: 1.85

Predicted: 1.25