

Anhydromethylenecitric acid
144-16-1 | DTXSID60162592

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.72e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.00e-01

Confidence level: 3.38e-01

Nearest Neighbors from the Training Set

Image not found

Furalaxyl

Measured: 1.13e-06

Predicted: 3.22e-07

Image not found

Oxalic acid

Measured: 1.57e-10

Predicted: 3.33e-04

Image not found

2,4,5-Trimethylphenol

Measured: 7.50e-08

Predicted: 1.72e-02

Image not found

Isobenzan

Measured: 3.00e-03

Predicted: 3.89e-06

Image not found

2-[2-(Hexyloxy)ethoxy]ethanol

Measured: 4.65e-05

Predicted: 6.01e-03