

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.99e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.38e-01

Confidence level: 3.84e-01

Nearest Neighbors from the Training Set

Image not found

Propisochlor

Measured: 2.11e-08

Predicted: 1.55e-05

Image not found

N-Nitrosodimethylamine

Measured: 1.36e-06

Predicted: 3.96

Image not found

1,2,3,5-Tetrachloronaphthalene

Measured: 3.10e-10

Predicted: 9.72e-06

Image not found

Pyridate

Measured: 3.64e-07

Predicted: 1.89e-08

Image not found

Haloxypop-etotyl

Measured: 1.28e-05

Predicted: 2.32e-07