

Citric acid
77-92-9 | DTXSID3020332

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: 9.65e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.70e-01

Confidence level: 2.89e-01

Nearest Neighbors from the Training Set

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Perflutren

Measured: 1.66e-08

Predicted: 7890

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2,2,5,5-Tetramethylhexane

Measured: 9.80e-08

Predicted: 7.94

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Benz(a)anthracene

Measured: 1.97e-10

Predicted: 2.14e-08

Image not found

Lepidine

Measured: 8.02e-14

Predicted: 9.90e-03

Image not found

1,4-Benzenediamine, N-(2,4-dinitrophenyl)-

Measured: 3.28e-08

Predicted: 5.92e-11