

Aspirin
50-78-2 | DTXSID5020108

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.46e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Penicillic acid

Measured: 1.18e-01

Predicted: 1.39e-01

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4-Ethoxy-3-methyl-4-oxobut-2-enoate

Measured: 9.42e-02

Predicted: 1.51e-01

[Image not found](#)

Phenylalanine

Measured: 1.34e-01

Predicted: 3.30e-01

[Image not found](#)

Phenylalanine

Measured: 1.34e-01

Predicted: 3.30e-01

[Image not found](#)

D-Phenylalanine

Measured: 1.34e-01

Predicted: 3.30e-01

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(Cyclopentyloxy)acetic acid

Measured: 1.42e-01

Predicted: 1.96e-01