

Benzoic acid, 2-methoxy-
579-75-9 | DTXSID3060376

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: 1.27e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 7.99e-01

Nearest Neighbors from the Training Set

Image not found

(Cyclopentyloxy)acetic acid

Measured: 1.42e-01

Predicted: 1.96e-01

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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

Image not found

Penicillic acid

Measured: 1.18e-01

Predicted: 1.39e-01

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2-Propenoic acid, 3-(2-furanyl)-

Measured: 1.45e-02

Predicted: 3.48e-01

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Tranexamic acid

Measured: 1.06

Predicted: 1.29

