

4-Aminopyridine
504-24-5 | DTXSID0023870

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.17e-01

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 6.21e-01

Nearest Neighbors from the Training Set

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2-Pyrrolicarboxylic acid

Measured: 0.85

Predicted: 3.04e-02

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Allyl cyanide

Measured: 0.4

Predicted: 2.45e-01

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2-Pyridone

Measured: -0.580

Predicted: -0.347

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Furan-3-carboxamide

Measured: 0.09

Predicted: 1.66e-01