

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 18.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.03e-01

Confidence level: 6.82e-01

Nearest Neighbors from the Training Set

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3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

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1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

Pyridine

Measured: 39.8

Predicted: 20.1

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2,2'-Bioxirane

Measured: 2.51

Predicted: 4.97

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Benzamide

Measured: 28.8

Predicted: 29.7