

4-Methylbenzenesulfonic acid
104-15-4 | DTXSID0026701

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: 2.37 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.81e-01

Confidence level: 5.86e-01

Nearest Neighbors from the Training Set

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4-Methylbenzenesulfonic acid

Measured: 3.60

Predicted: 2.37

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Methanesulfonic acid

Measured: 10.4

Predicted: 6.76

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4-Aminobenzenesulfonic acid

Measured: 6.24e-02

Predicted: 1.78e-01

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2-Hydroxyethanesulfonic acid

Measured: 7.93

Predicted: 6.22

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Naphthalene-2-sulfonic acid

Measured: 3.26

Predicted: 1.08