

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 89.0 °C

Global applicability domain: Inside

Local applicability domain index: 7.73e-01

Confidence level: 6.81e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Methylbenzenesulfonic acid

Measured: 105

Predicted: 89.0

[Image not found](#)

Benzenesulfonic acid

Measured: 65.0

Predicted: 72.2

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2,4-Dimethylbenzenesulfonic acid

Measured: 57.0

Predicted: 68.6

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Benzenesulfonic acid

Measured: 84.0

Predicted: 85.4