

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.19e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.94e-01

Confidence level: 3.33e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methenamine

Measured: 5.25e-05

Predicted: 8.35e-03

[Image not found](#)

p-Phenylazophenol

Measured: 4.72e-08

Predicted: 5.18e-07

[Image not found](#)

Formetanate hydrochloride

Measured: 1.50e-07

Predicted: 1.86e-07

[Image not found](#)

Pyrethrin II

Measured: 1.04e-05

Predicted: 3.95e-07