

4-Methylbenzenesulfonic acid
104-15-4 | DTXSID0026701

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 292 °C

Global applicability domain: Outside

Local applicability domain index: 2.15e-01

Confidence level: 5.17e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 2,4,5-trimethoxy-

Measured: 300

Predicted: 302

Image not found

Dimethyl phosphate

Measured: 174

Predicted: 181

Image not found

Trimellitic anhydride

Measured: 390

Predicted: 366

Image not found

2-Benzofurancarboxylic acid

Measured: 313

Predicted: 303

Image not found

MCPA

Measured: 287

Predicted: 278