

Methanesulfonic acid
75-75-2 | DTXSID4026422

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: 1.37e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.64e-01

Confidence level: 5.19e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Propylene oxide

Measured: 4.28e-04

Predicted: 548

Image not found

Butane, 1-methoxy-

Measured: 3.41e-03

Predicted: 138

Image not found

Propyl acetate

Measured: 8.02e-02

Predicted: 34.1

Image not found

1-Chloropropan-2-one

Measured: 1.19e-01

Predicted: 33.9

Image not found

2,2-Dimethylpropanol

Measured: 3.41e-01

Predicted: 9.65