

Sodium 3-nitrobenzenesulfonate
127-68-4 | DTXSID2027048

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: 2.27e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.33e-01

Confidence level: 3.96e-01

Nearest Neighbors from the Training Set

Image not found

3,5-Dichlorodiphenyl ether

Measured: 3.45e-06

Predicted: 9.56e-04

Image not found

Aldicarb sulfoxide

Measured: 9.00e-05

Predicted: 6.19e-05

Image not found

Orbencarb

Measured: 2.00e-06

Predicted: 1.81e-05