

Octaneperoxoic acid
33734-57-5 | DTXSID7074618

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: 6.53e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 4.66e-01

Nearest Neighbors from the Training Set

Image not found

1-Naphthylamine

Measured: 4.00e-01

Predicted: 9.37e-04

Image not found

2-Butanone, 1-bromo-

Measured: 1.26e-01

Predicted: 7.89

Image not found

Phenyl phosphorodichloridate

Measured: 5.23e-02

Predicted: 1.16e-02

Image not found

Nonylamine

Measured: 1.55e-01

Predicted: 2.75e-01

Image not found

2,2,3,3-Tetramethylpentane

Measured: 1.37e-03

Predicted: 13.5