

8-Hydroxyoctanoic acid
764-89-6 | DTXSID40227234

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: 1.89e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.21e-01

Confidence level: 4.26e-01

Nearest Neighbors from the Training Set

Image not found

Cycloheptanone

Measured: 2.88e-07

Predicted: 1.00

Image not found

Piperazine

Measured: 9.00e-08

Predicted: 7.31e-01

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3-Methylbutyl acetate

Measured: 1.07e-08

Predicted: 6.64

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Diallylamine

Measured: 3.18e-07

Predicted: 27.5

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Pentan-2-ol

Measured: 3.14e-06

Predicted: 5.03