

Deacetylmoxisylyte
35231-36-8 | DTXSID10188722

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: 7.85e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.84e-01

Confidence level: 6.22e-01

Nearest Neighbors from the Training Set

Image not found

Chlorpropham

Measured: 3.80e-07

Predicted: 1.18e-04

Image not found

4-Penten-2-one, 4-methyl-

Measured: 1.42e-04

Predicted: 11.7

Image not found

Anilazine

Measured: 1.80e-04

Predicted: 3.20e-08

Image not found

Trimethoxysilane

Measured: 3.00e-05

Predicted: 50.9

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2,4-Dichlorophenoxyacetic acid

Measured: 4.33e-07

Predicted: 7.12e-07