

Chloralose
15879-93-3 | DTXSID4020088

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: 6.57e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.98e-01

Confidence level: 4.82e-01

Nearest Neighbors from the Training Set

Image not found

2,4,5-Trimethylphenol

Measured: 7.50e-08

Predicted: 1.72e-02

Image not found

Isobenzan

Measured: 3.00e-03

Predicted: 3.89e-06

Image not found

Crotoxyphos

Measured: 1.28e-04

Predicted: 1.33e-05

Image not found

2-[2-(Hexyloxy)ethoxy]ethanol

Measured: 4.65e-05

Predicted: 6.01e-03

Image not found

Hexythiazox

Measured: 1.01e-08

Predicted: 2.42e-08