

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.69e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.40e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

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2-[bis(2-cyanoethyl)amino]-4-methylsulfanylbutanoic acid

Measured: 4.70e-02

Predicted: 7.00e-02

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2',3'-Dideoxycytidine

Measured: 3.62e-01

Predicted: 3.46e-01

[Image not found](#)

Dexpanthenol

Measured: 4.87

Predicted: 3.46