

Chloral
75-87-6 | DTXSID7024744

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 8.51 days

Global applicability domain: Outside

Local applicability domain index: 4.09e-01

Confidence level: 7.51e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethylcyclopentane

Measured: 511

Predicted: 8.14

[Image not found](#)

Pentane

Measured: 40.7

Predicted: 6.52

[Image not found](#)

n-Hexane

Measured: 157

Predicted: 7.45

[Image not found](#)

Heptane

Measured: 88.3

Predicted: 7.54

[Image not found](#)

Octane

Measured: 157

Predicted: 8.57