

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 314 °C

Global applicability domain: Outside

Local applicability domain index: 2.02e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

Image not found

Pyrogallol

Measured: 309

Predicted: 292

Image not found

4-Hexylresorcinol

Measured: 334

Predicted: 302

Image not found

(1,1'-Biphenyl)-2,2'-diol

Measured: 320

Predicted: 315

Image not found

Triisopropanolamine

Measured: 305

Predicted: 302