

Chloral  
75-87-6 | DTXSID7024744

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
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.64 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.94 \times 10^{-1}$

**Confidence level:**  $8.70 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

Chloral

**Measured:**  $1.60 \times 10^{-12}$

**Predicted:**  $1.64 \times 10^{-12}$

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Dichloroacetaldehyde

**Measured:**  $2.30 \times 10^{-12}$

**Predicted:**  $2.47 \times 10^{-12}$

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Trichloroethylene

**Measured:**  $2.36 \times 10^{-12}$

**Predicted:**  $2.21 \times 10^{-12}$