

Hexachloro-1,3-butadiene  
87-68-3 | DTXSID7020683

### 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:** 1.79e-05 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 6.76e-01

**Confidence level:** 5.71e-01

## Nearest Neighbors from the Training Set

Image not found

Hexachloro-1,3-butadiene

**Measured:** 1.23e-05

**Predicted:** 1.79e-05

Image not found

Hexachlorocyclopentadiene

**Measured:** 6.60e-06

**Predicted:** 9.10e-06

Image not found

Hexachloropropene

**Measured:** 6.84e-05

**Predicted:** 2.12e-04

Image not found

Carbon tetrabromide

**Measured:** 7.24e-04

**Predicted:** 8.16e-04

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Propane, 1,3-dibromo-2,2-bis(bromomethyl)-

**Measured:** 4.13e-06

**Predicted:** 7.44e-06