

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3610

Global applicability domain: Inside

Local applicability domain index: 5.79e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Hexachloro-1,3-butadiene

Measured: 6610

Predicted: 3610

[Image not found](#)

Hexachloroethane

Measured: 513

Predicted: 452

[Image not found](#)

Kepone

Measured: 1550

Predicted: 1380

[Image not found](#)

Tetrachloroethylene

Measured: 52.5

Predicted: 42.2