

Isophorone  
78-59-1 | DTXSID8020759

### 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
0.91	1.08	0.91	1.08	0.92	1.00

## Model Results

**Predicted value:** 5.79e-01 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 7.21e-01

**Confidence level:** 7.38e-01

## Nearest Neighbors from the Training Set

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Menazon

**Measured:** 4.38e-01

**Predicted:** 3.69e-07

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Isovaleric acid

**Measured:** 2.77e-01

**Predicted:** 3.57e-01

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1,2-Butadiene

**Measured:** 1.50

**Predicted:** 905

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4-Propylphenol

**Measured:** 1.28

**Predicted:** 3.72e-02

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4-Bromobenzoic acid

**Measured:** 1.50

**Predicted:** 4.93e-05