

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
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 3.19

**Global applicability domain:** Inside

**Local applicability domain index:** 5.84e-01

**Confidence level:** 5.93e-01

## Nearest Neighbors from the Training Set

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Isophorone

**Measured:** 2.00

**Predicted:** 3.19

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Triallylamine

**Measured:** 3.55

**Predicted:** 4.23

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N,N-Dimethyl-1,2-dithiolan-4-amine

**Measured:** 52.5

**Predicted:** 17.5

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Triethylamine

**Measured:** 4.90

**Predicted:** 5.95

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O,O-Diethyl dithiophosphate

**Measured:** 5.01

**Predicted:** 5.43