

Thiamine disulfide  
67-16-3 | DTXSID6046890

### 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:** 8.69e-03 mol/L

**Global applicability domain:** Outside

**Local applicability domain index:** 1.99e-01

**Confidence level:** 7.49e-01

## Nearest Neighbors from the Training Set

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Aconitine

**Measured:** 4.80e-04

**Predicted:** 8.92e-04

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Psicofuranine

**Measured:** 2.69e-02

**Predicted:** 3.98e-02

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Cephadrine

**Measured:** 6.10e-02

**Predicted:** 6.70e-02

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Cefaclor

**Measured:** 2.72e-02

**Predicted:** 7.84e-02