

Triisopropanolamine  
122-20-3 | DTXSID5021415

### Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

#### 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:** 3.33 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 4.67e-01

**Confidence level:** 7.12e-01

## Nearest Neighbors from the Training Set

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Triisopropanolamine

**Measured:** 4.34

**Predicted:** 3.33

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Triethanolamine

**Measured:** 6.70

**Predicted:** 6.72

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2-[bis(2-cyanoethyl)amino]propanoic acid

**Measured:** 6.66e-01

**Predicted:** 5.69e-01

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Dexpanthenol

**Measured:** 4.87

**Predicted:** 3.46