

5-Ethyl-1-methyl-5-(1-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione  
61346-87-0 | DTXSID60818264

### Model Performance

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

#### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.85            | 1.14 | 0.85           | 1.12 | 0.83       | 1.23 |

## Model Results

**Predicted value:** 2.96e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 1.21e-01

**Confidence level:** 6.39e-01

## Nearest Neighbors from the Training Set

Image not found

2-Methyl-p-benzoquinone

**Measured:** 2.35e-11

**Predicted:** 2.15e-11

Image not found

1,4-Naphthoquinone

**Measured:** 3.10e-12

**Predicted:** 3.16e-11