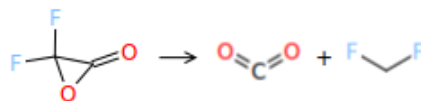


## 2 reactions matched to 1+2\_Cycloaddition

index: 23



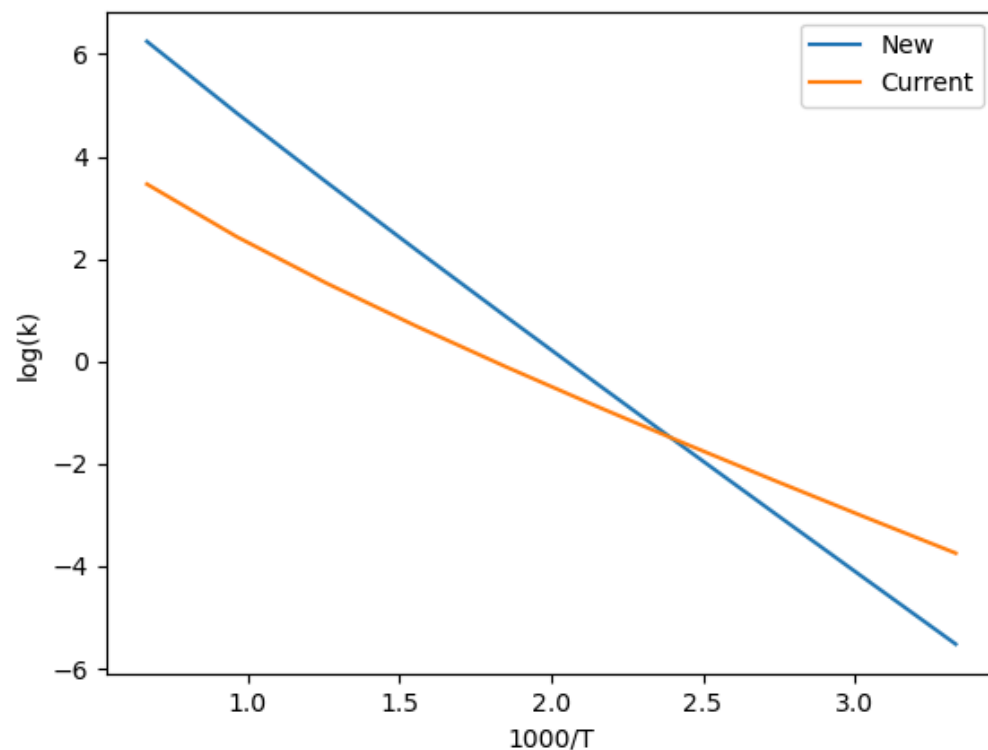
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

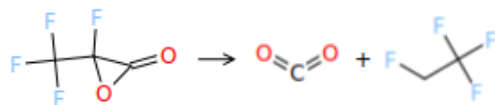
Arrhenius( $A=(273000, \text{'s}^{-1}\text{'})$ ,  $n=1.12$ ,  $E_a=(18850, \text{'cal/mol}\text{'})$ ,  $T_0=(1, \text{'K}\text{'})$ )

**Current Kinetics**

ArrheniusEP( $A=(96.315, \text{'cm}^3/(\text{mol}\cdot\text{s})\text{'})$ ,  $n=2.76922$ ,  $\alpha=0$ ,  $E_0=(37839.3, \text{'J/mol}\text{'})$ ,  $T_{\min}=(298, \text{'K}\text{'})$ ,  $T_{\max}=(2500, \text{'K}\text{'})$ ,  $\text{comment}=""$  "Average of [From training reaction 18 used for CF<sub>2</sub>;mb\_carbonyl\_2H] Estimated using an average for rate rule [CF<sub>2</sub>;mb\_carbonyl] Euclidian distance = 0 Multiplied by reaction path degeneracy 2.0 family: 1+2\_Cycloaddition"")



index: 63



**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

Arrhenius( $A=(2.31 \times 10^{27}, \text{s}^{-1})$ ,  $n=-5.84$ ,  $E_a=(33140, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

**Current Kinetics**

ArrheniusEP( $A=(9.6315 \times 10^{-5}, \text{m}^3/(\text{mol} \cdot \text{s}))$ ,  $n=2.76922$ ,  $\alpha=0$ ,  $E_0=(37.8393, \text{kJ/mol})$ ,  $\text{comment}=""$  Average of [Average of [Average of [From training reaction 18 used for CF2;mb\_carbonyl\_2H] + Average of [From training reaction 18 used for CF2;mb\_carbonyl\_2H]] + Average of [Average of [From training reaction 18 used for CF2;mb\_carbonyl\_2H]]] Estimated using template [elec\_def;mb\_carbonyl] for rate rule [me\_carbene;mb\_carbonyl] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1+2\_Cycloaddition""")

