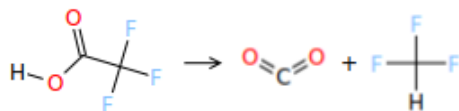


## 9 reactions matched to 1,3\_Insertion\_CO2

index: 27



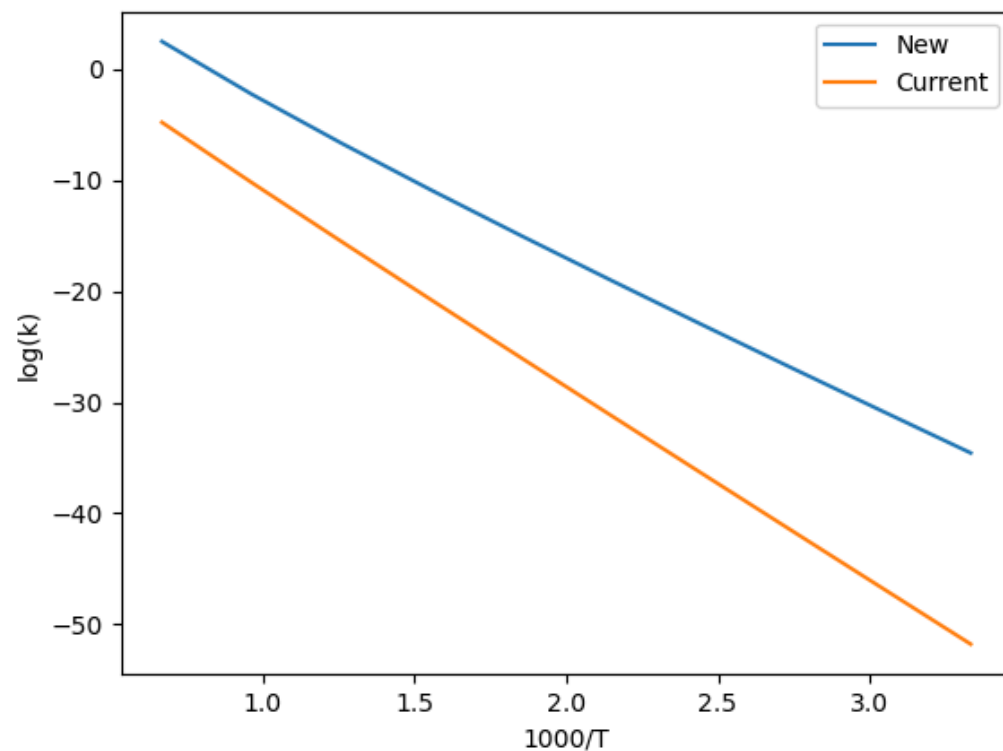
Note: Training reaction written in opposite direction from reaction family.

**New Kinetics:**

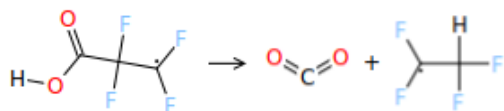
Arrhenius( $A=(5.08 \times 10^{-15}, \text{s}^{-1})$ ,  $n=7.77$ ,  $E_a=(54250, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

**Current Kinetics**

ArrheniusEP( $A=(0.0347248, \text{m}^3/(\text{mol} \cdot \text{s}))$ ,  $n=2.50667$ ,  $\alpha=0$ ,  $E_0=(324.678, \text{kJ/mol})$ ,  $\text{comment}=""$  Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



index: 66



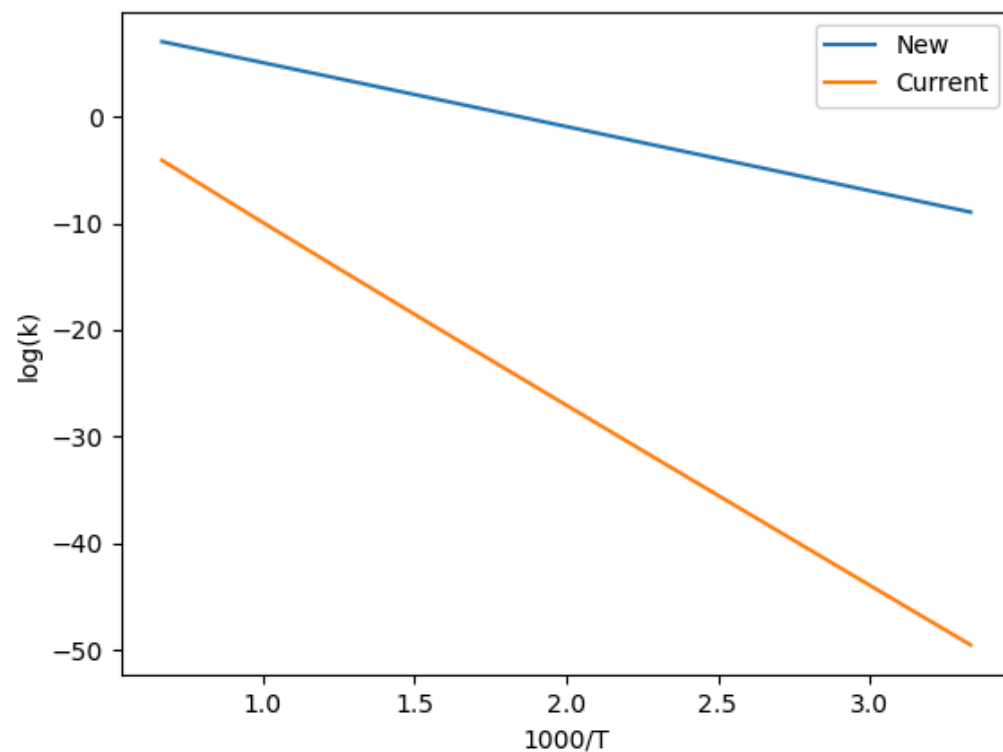
Note: Training reaction written in opposite direction from reaction family.

**New Kinetics:**

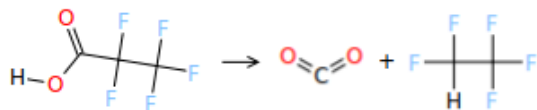
Arrhenius( $A=(7.38e+11, 's^{-1}')$ ,  $n=-0.25$ ,  $E_a=(27740, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

**Current Kinetics**

ArrheniusEP( $A=(10.2406, 'm^3/(mol*s)')$ ,  $n=1.86833$ ,  $\alpha=0$ ,  $E_0=(316.938, 'kJ/mol')$ ,  $comment=""$  Average of [From training reaction 1 used for CO2\_Cdd;H2 + Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using an average for rate rule [CO2\_Cdd;R\_H] Euclidian distance = 0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



index: 70



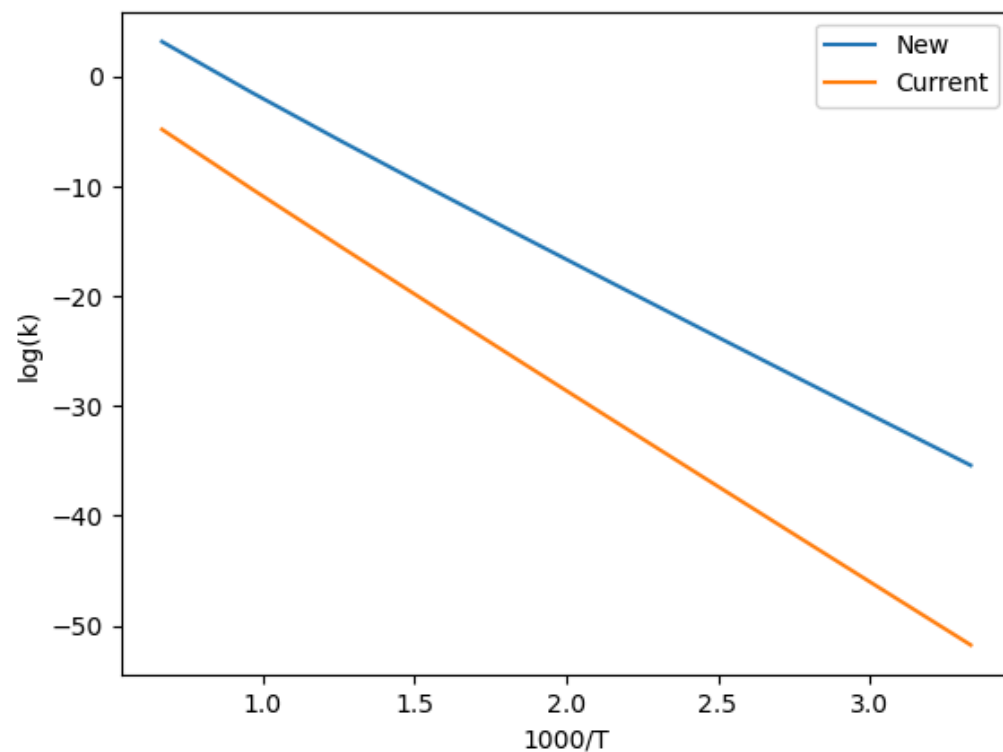
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

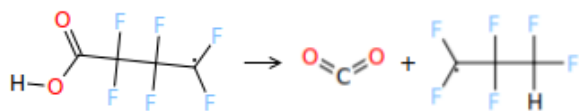
Arrhenius( $A=(0.0468, \text{s}^{-1})$ ,  $n=4.23$ ,  $E_a=(61170, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

**Current Kinetics**

ArrheniusEP( $A=(0.0347248, \text{m}^3/(\text{mol}\cdot\text{s}))$ ,  $n=2.50667$ ,  $\alpha=0$ ,  $E_0=(324.678, \text{kJ/mol})$ ,  $\text{comment}=""$  Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



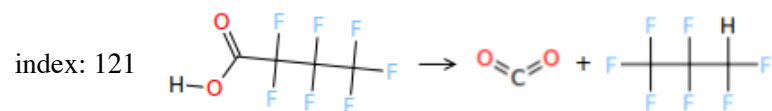
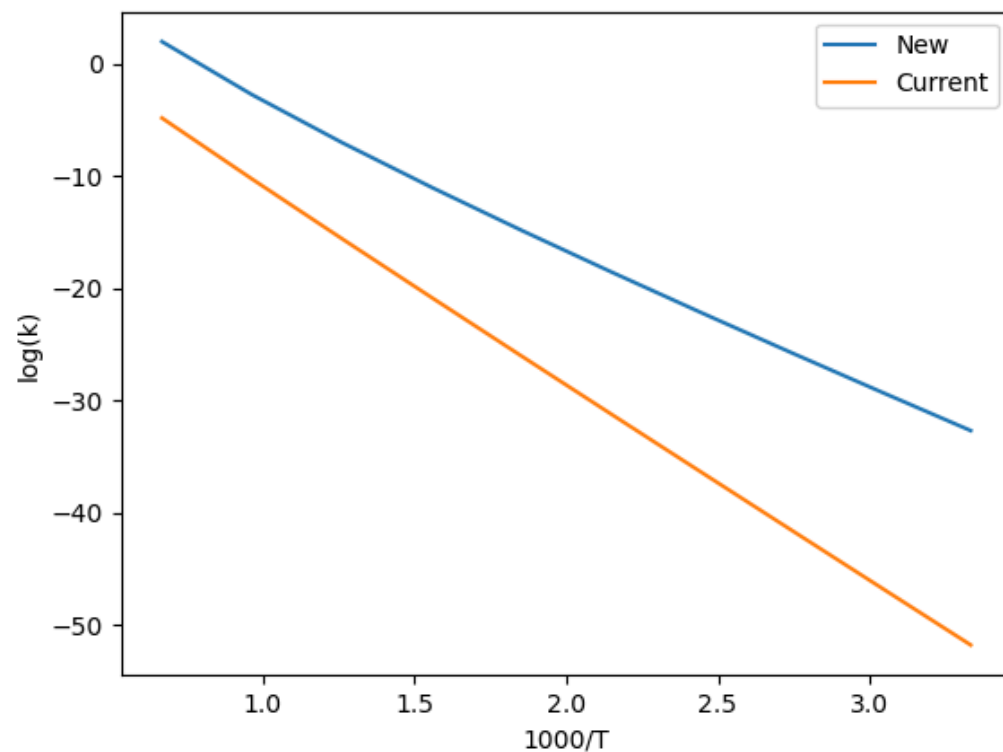
index: 116



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

## Arrhenius(A=(1.67e-25,'s^-1'), n=10.58, Ea=(46810,'cal/mol'), T0=(1,'K'))

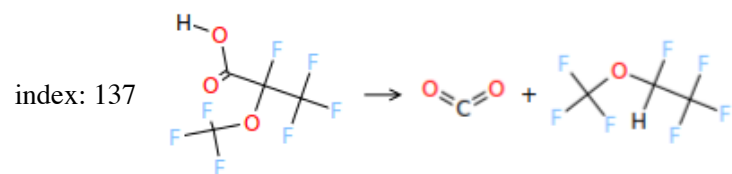
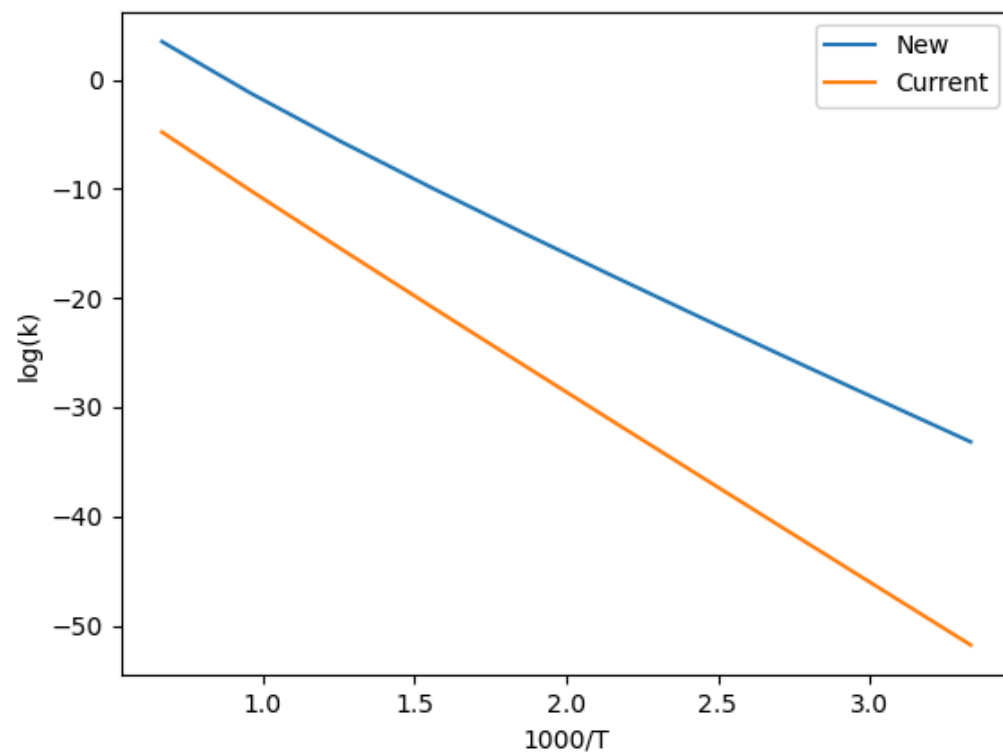
ArrheniusEP(A=(0.0347248,'m^3/(mol\*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment=""Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



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

## Arrhenius(A=(5.74e-17,'s^-1'), n=8.62, Ea=(52560,'cal/mol'), T0=(1,'K'))

ArrheniusEP(A=(0.0347248,'m^3/(mol\*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment=""Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



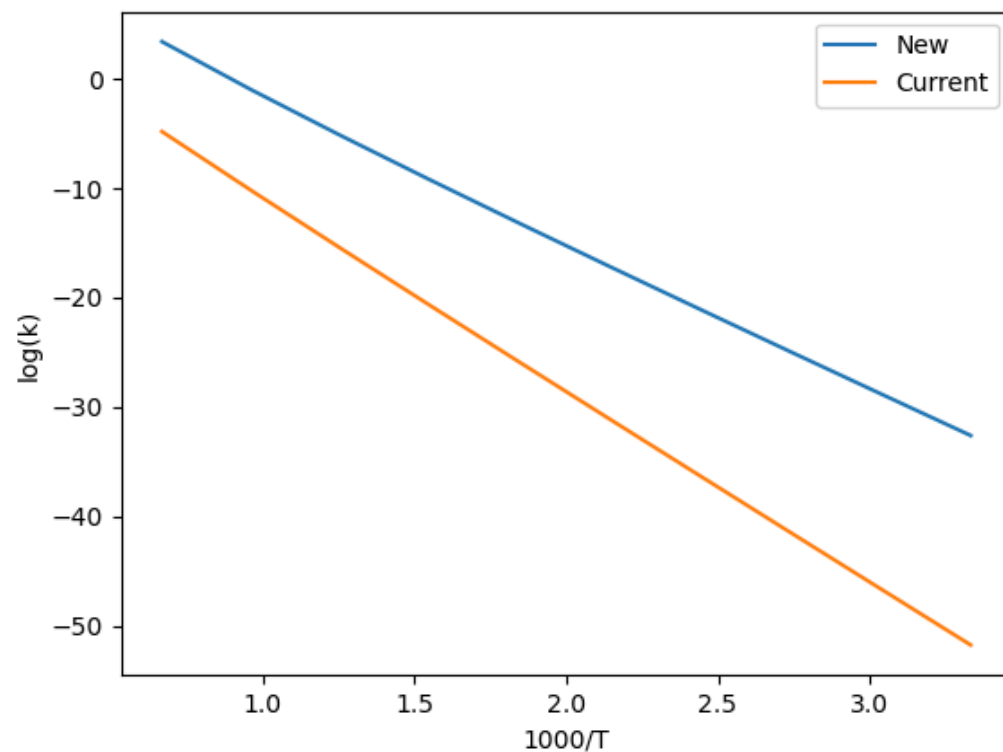
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

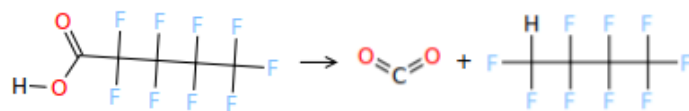
Arrhenius( $A=(9.42\text{e-}06, \text{'s}^{-1}\text{'})$ ,  $n=5.21$ ,  $E_a=(55590, \text{'cal/mol'})$ ,  $T_0=(1, \text{'K'})$ )

**Current Kinetics**

ArrheniusEP( $A=(0.0347248, \text{'m}^3/(\text{mol}\cdot\text{s})\text{'})$ ,  $n=2.50667$ ,  $\alpha=0$ ,  $E_0=(324.678, \text{'kJ/mol'})$ ,  $\text{comment}=""$  Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



index: 163



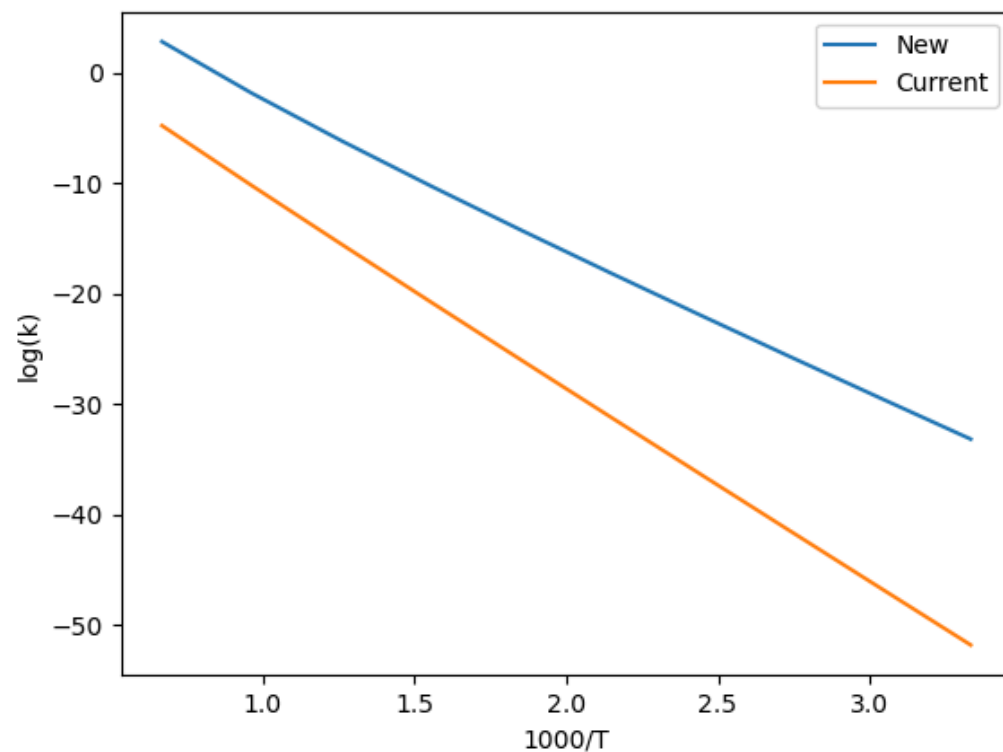
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

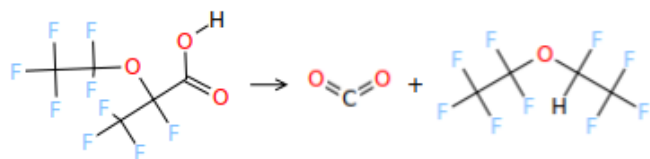
Arrhenius( $A=(2.52\text{e-}16, \text{'s}^{-1})$ ,  $n=8.17$ ,  $E_a=(51890, \text{'cal/mol'})$ ,  $T_0=(1, \text{'K'})$ )

**Current Kinetics**

ArrheniusEP( $A=(0.0347248, \text{'m}^3/(\text{mol*s})$ '),  $n=2.50667$ ,  $\alpha=0$ ,  $E_0=(324.678, \text{'kJ/mol'})$ ,  $\text{comment}=""$  Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



index: 179



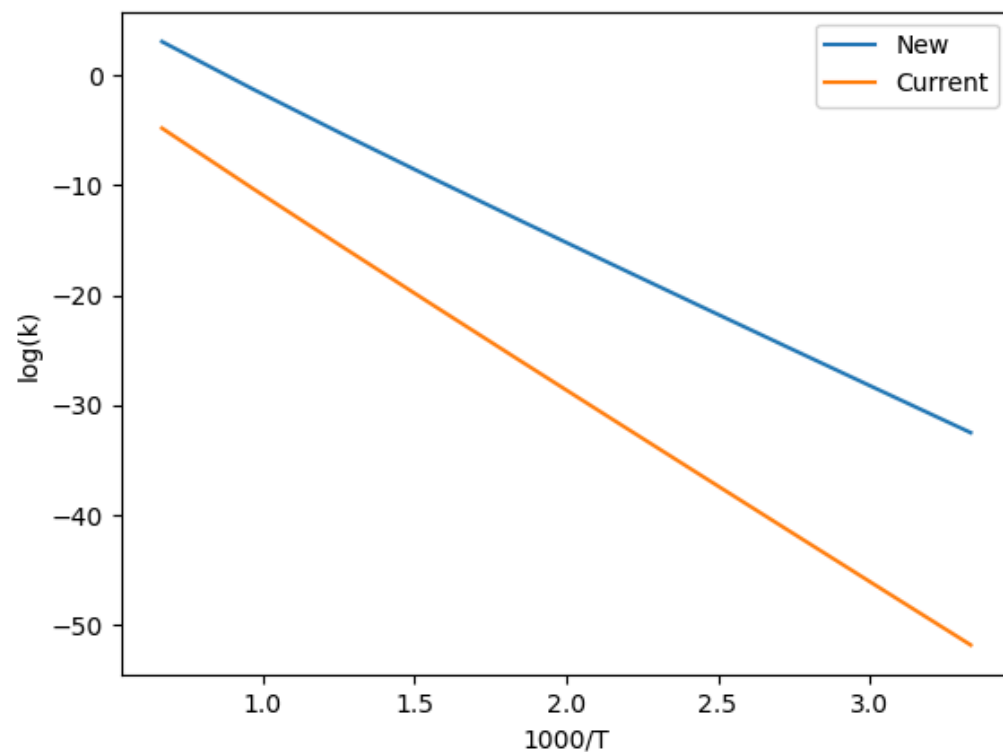
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

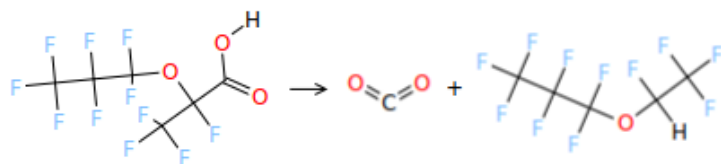
Arrhenius( $A=(0.0958, \text{s}^{-1})$ ,  $n=3.87$ ,  $E_a=(56350, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

**Current Kinetics**

ArrheniusEP( $A=(0.0347248, \text{m}^3/(\text{mol}\cdot\text{s}))$ ,  $n=2.50667$ ,  $\alpha=0$ ,  $E_0=(324.678, \text{kJ/mol})$ ,  $\text{comment}=""$  Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")



index: 191



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



**New Kinetics:**

Arrhenius( $A=(7.25\text{e-}14, \text{'s}^{-1}\text{'})$ ,  $n=7.69$ ,  $E_a=(51640, \text{'cal/mol'})$ ,  $T_0=(1, \text{'K'})$ )

**Current Kinetics**

ArrheniusEP( $A=(0.0347248, \text{'m}^3/(\text{mol}\cdot\text{s})\text{'})$ ,  $n=2.50667$ ,  $\alpha=0$ ,  $E_0=(324.678, \text{'kJ/mol'})$ ,  $\text{comment}=""$  "Average of [From training reaction 2 used for CO2\_Cdd;C\_methane + Average of [From training reaction 3 used for CO2\_Cdd;C\_pri/NonDeC] + Average of [From training reaction 4 used for CO2\_Cdd;C/H2/NonDeC]] Estimated using template [CO2\_Cdd;Cs\_H] for rate rule [CO2\_Cdd;C\_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3\_Insertion\_CO2""")

