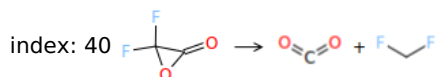


2 reactions matched to 1+2_Cycloaddition



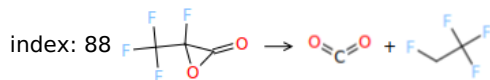
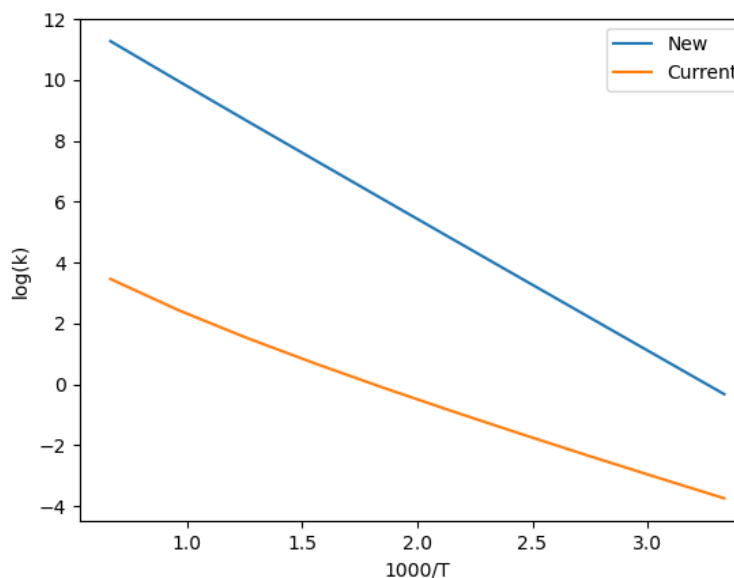
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.17e+13, 's^{-1}')$, $n=0.33$, $E_a=(19504.5, 'cal/mol')$, $T_0=(1, 'K')$)

Current Kinetics

ArrheniusEP($A=(96.315, 'cm^3/(mol*s)')$, $n=2.76922$, $\alpha=0$, $E_0=(37839.3, 'J/mol')$, $T_{min}=(298, 'K')$, $T_{max}=(2500, 'K')$, $comment=""$ "Average of [From training reaction 18 used for CF2;mb_carbonyl_2H] Estimated using an average for rate rule [CF2;mb_carbonyl] Euclidian distance = 0 Multiplied by reaction path degeneracy 2.0 family: 1+2_Cycloaddition")



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

New Kinetics:

Arrhenius($A=(3.81e+12, 's^{-1}')$, $n=0.64$, $E_a=(32162.9, 'cal/mol')$, $T_0=(1, 'K')$)

Current Kinetics

ArrheniusEP($A=(9.6315e-05, 'm^3/(mol*s)')$, $n=2.76922$, $\alpha=0$, $E_0=(37.8393, 'kJ/mol')$, $comment=""$ "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")

