## 14 reactions matched to R\_Addition\_MultipleBond

index: 4 
$$F \xrightarrow{F} 0 \cdot \rightarrow F \xrightarrow{F} 0 + F \cdot$$

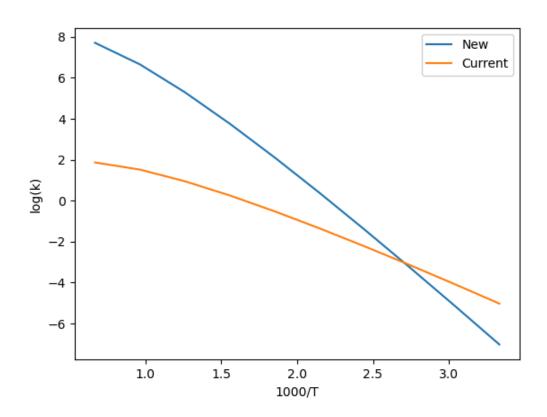
Note: Training reaction written in opposite direction from reaction family.

### **New Kinetics:**

Arrhenius(A=(1.81e+35,'s^-1'), n=-7.12, Ea=(33830,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

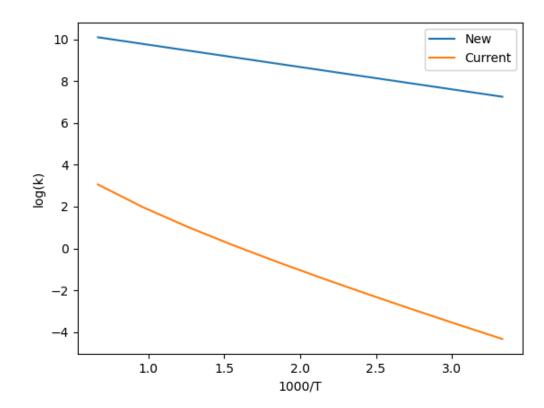
 $\label{eq:local_symmetric} Arrhenius BM(A=(4.08261e+20,'m^3/(mol^*s)'), n=-5.07836, w0=(384,'kJ/mol'), E0=(74.9893,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-3R-inRing_N-3R-C_N-1R!H->N_2R!H->O',), comment="""Estimated from node Root_N-3R-inRing_N-3R->C_N-1R!H->N_2R!H->O""")$ 



Arrhenius(A=(6.32e+10,'s^-1'), n=0, Ea=(4872,'cal/mol'), T0=(1,'K'))

## **Current Kinetics**

ArrheniusBM(A=(1.4291e-06,'m^3/(mol\*s)'), n=3.20779, w0= (393.5,'kJ/mol'), E0=(36.9032,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R N-Sp-4R!H=3R 3R->C Ext-1R!H-R N-5R!H-inRing Ext-1R!H-R\_N-2R!H->C\_N-5R!H-u1',), comment="""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!HinRing\_Ext-1R!H-R\_N-2R!H->C\_N-5R!H-u1""")

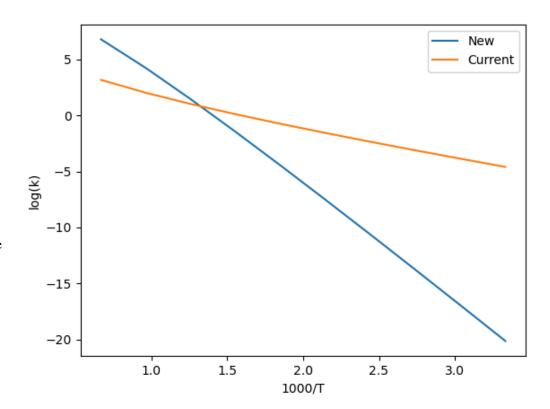


index: 32 
$$\stackrel{\mathsf{F}}{\triangleright} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\triangleright} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}$$

Arrhenius(A=(1.01e+31,'s^-1'), n=-5.22, Ea=(52440,'cal/mol'), T0=(1,'K'))

## **Current Kinetics**

ArrheniusBM(A=(1.89178e-07,'m^3/(mol\*s)'), n=3.53001, w0= (303.056,'kJ/mol'), E0=(38.0148,'kJ/mol'), Tmin=(300,'K'), Tmax= (2000,'K'), uncertainty=RateUncertainty(mu=-0.4944253016374622, var=1.7828810760479818, Tref=1000.0, N=135, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!H-inRing\_Ext-1R!H-R',), comment="""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!H-inRing\_Ext-1R!H-R Multiplied by reaction path degeneracy 2.0""")

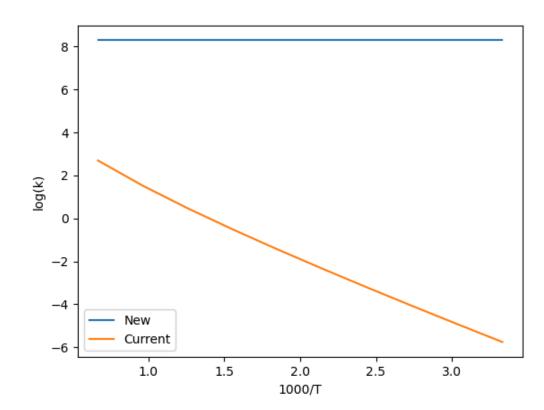


index: 51 
$$F \stackrel{F}{=} F \stackrel{F}{=} O \cdot \longrightarrow F \stackrel{O}{=} F \stackrel{F}{=} F$$

 $Arrhenius(A=(1.95e+08, 's^{\Lambda}-1'), n=0, Ea=(0, 'cal/mol'), T0=(1, 'K'))$ 

## **Current Kinetics**

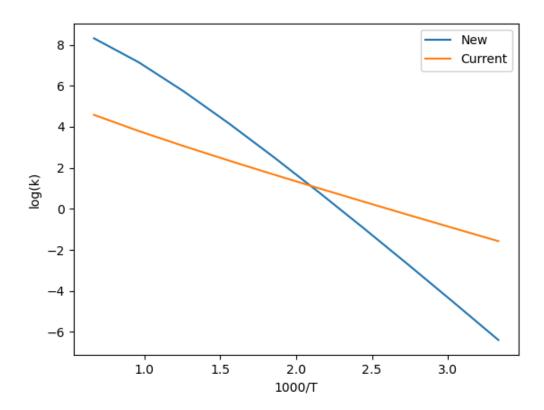
 $\label{eq:approx} Arrhenius BM(A=(1.22525e-05,'m^3/(mol^*s)'), n=2.9005, w0=(393.5,'kJ/mol'), E0=(46.1097,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_N-Sp-5R!H=4R!H_Sp-2R!H=1R!H_Ext-4R!H-R_N-2R!H->C',), comment="""Estimated from node Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_N-Sp-5R!H=4R!H_Sp-2R!H=1R!H_Ext-4R!H-R_N-2R!H->C'"")$ 



Arrhenius(A=(6.11e+30,'s^-1'), n=-5.61, Ea=(31960,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

 $\label{eq:arrhenius} Arrhenius BM(A=(61.188,'m^3/(mol^*s)'), n=1.29312, w0=(297.108,'kJ/mol'), E0=(37.7031,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.28976280499384915, var=2.1569028208455543, Tref=1000.0, N=37, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_N-Sp-4R!H=3R_3R->C_Ext-3C-R_2R!H->C',), comment="""Estimated from node Root_N-3R-inRing_Ext-3R-R_N-Sp-4R!H=3R_3R->C_Ext-3C-R_2R!H->C""")$ 

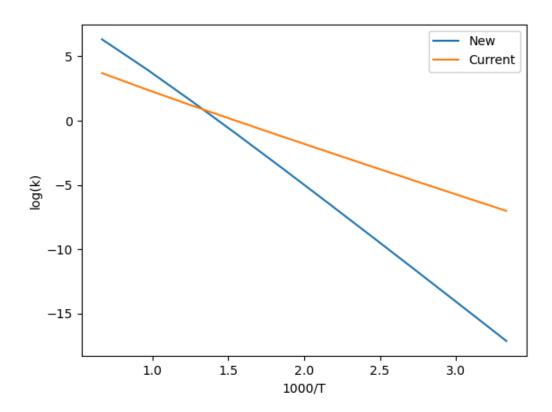


index: 65 
$$\stackrel{\text{HO}}{\longrightarrow}$$
  $\stackrel{\text{F}}{\longleftarrow}$   $\stackrel{\text{F}}{\longleftarrow}$   $\stackrel{\text{F}}{\longrightarrow}$   $\stackrel{\text{F}}{\longleftarrow}$   $\stackrel{\text{CH}}{\longleftarrow}$   $\stackrel{\text{OH}}{\longrightarrow}$ 

Arrhenius(A=(1.42e+23,'s^-1'), n=-3.27, Ea=(44170,'cal/mol'), T0=(1,'K'))

## **Current Kinetics**

 $\label{eq:analytime} Arrhenius BM(A=(306.062,'m^3/(mol^*s)'), n=1.16366, w0=(301.402,'kJ/mol'), E0=(71.0975,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.022037706214473284, var=2.370141635838845, Tref=1000.0, N=230, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Sp-4R!H=3R_Sp-2R!H=1R!H',), comment=""Estimated from node Root_N-3R-inRing_Ext-3R-R_Sp-4R!H=3R_Sp-2R!H=1R!H Multiplied by reaction path degeneracy 2.0""")$ 

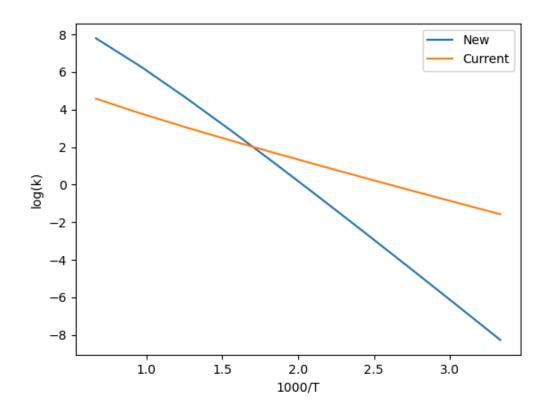


index: 75 
$$\stackrel{\mathsf{F}}{\underset{\mathsf{F}}{\bigvee}} \overset{\mathsf{O}}{\underset{\mathsf{OH}}{\bigvee}} \to \overset{\mathsf{HO}}{\underset{\mathsf{O}}{\bigvee}} \overset{\mathsf{F}}{\underset{\mathsf{F}}{\bigvee}} + \overset{\mathsf{F}}{\underset{\mathsf{F}}{\bigvee}} \overset{\mathsf{F}}{\underset{\mathsf{F}}{\bigvee}}$$

Arrhenius(A=(1.18e+23,'s^-1'), n=-3.36, Ea=(31600,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(61.188,'m^3/(mol\*s)'), n=1.29312, w0= (297.108,'kJ/mol'), E0=(37.7031,'kJ/mol'), Tmin=(300,'K'), Tmax= (2000,'K'), uncertainty=RateUncertainty(mu=-0.28976280499384915, var=2.1569028208455543, Tref=1000.0, N=37, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C',), comment="""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C""")

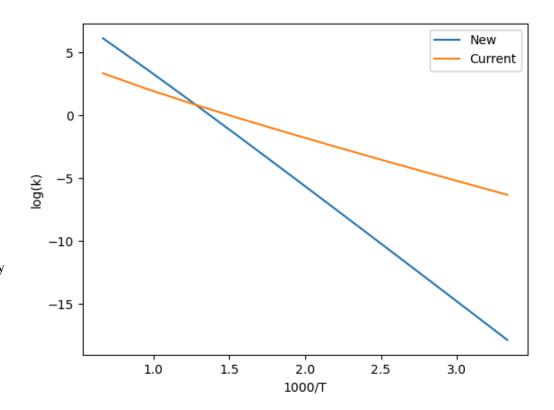


index: 78 
$$\stackrel{\mathsf{F}}{\triangleright} \stackrel{\mathsf{F}}{\models} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{$$

Arrhenius(A=(1.4e+18,'s^-1'), n=-1.79, Ea=(43360,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

 $\label{eq:analytical_armonius_bm} Arrhenius_{M}(A=(0.00504,\text{'m}^3/(\text{mol*s})'), n=2.41, w0=(301,\text{'kJ/mol'}), E0=(57.3723,\text{'kJ/mol'}), Tmin=(300,\text{'K'}), Tmax=(2000,\text{'K'}), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_N-Sp-5R!H=4R!H_Sp-2R!H=1R!H_Ext-4R!H-R_2R!H->C',), comment=""Estimated from node Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_N-Sp-5R!H=4R!H_Sp-2R!H=1R!H_Ext-4R!H-R_2R!H->C Multiplied by reaction path degeneracy 2.0""")$ 

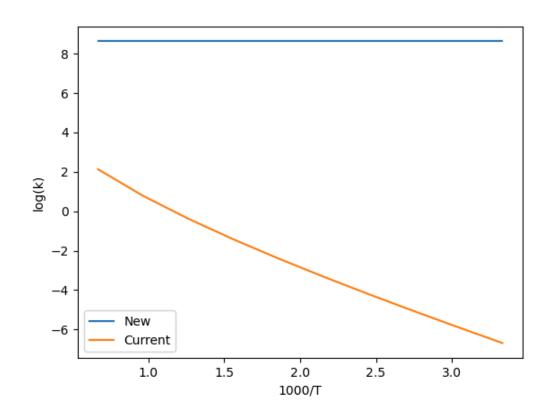


index: 100 
$$F = F = F = F = F$$

 $Arrhenius(A = (4.3e + 08, 's^{-1}), n = 0, Ea = (0, 'cal/mol'), T0 = (1, 'K'))$ 

## **Current Kinetics**

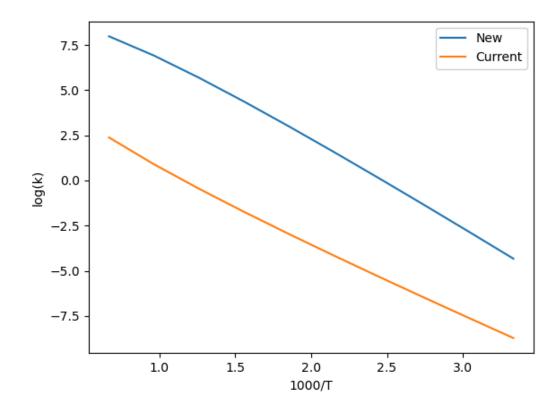
 $\label{eq:approx} Arrhenius BM(A=(2.13223e-11,'m^3/(mol^*s)'), n=4.48095, w0=(299.5,'kJ/mol'), E0=(40.9045,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.6004730311185978, var=1.5705211473983438, Tref=1000.0, N=276, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_Ext-3R-R_Ext-1R!H-R_N-8R!H-inRing',), comment="""Estimated from node Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_Ext-1R!H-R_N-8R!H-inRing""")$ 



Arrhenius(A=(2.62e+23,'s^-1'), n=-3.69, Ea=(25540,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(9.07578e-06,'m^3/(mol\*s)'), n=3.04336, w0= (299.503,'kJ/mol'), E0=(64.4187,'kJ/mol'), Tmin=(300,'K'), Tmax= (2000,'K'), uncertainty=RateUncertainty(mu=-0.3757377757886876, var=2.242054186761003, Tref=1000.0, N=1042, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R',), comment="""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R""")

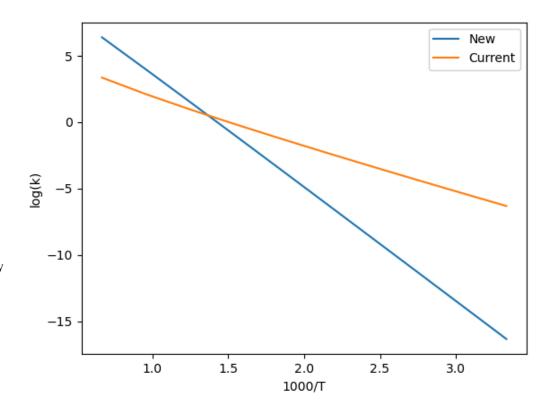


index: 115 
$$\stackrel{\text{HO}}{\longrightarrow}$$
  $\stackrel{\text{F}}{\longrightarrow}$   $\stackrel{\text{F}}{\longrightarrow}$   $\stackrel{\text{F}}{\longrightarrow}$   $\stackrel{\text{F}}{\longrightarrow}$   $\stackrel{\text{F}}{\longrightarrow}$   $\stackrel{\text{HO}}{\longrightarrow}$   $\stackrel{\text{F}}{\longrightarrow}$ 

Arrhenius(A=(1.68e+14,'s^-1'), n=-0.64, Ea=(39780,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

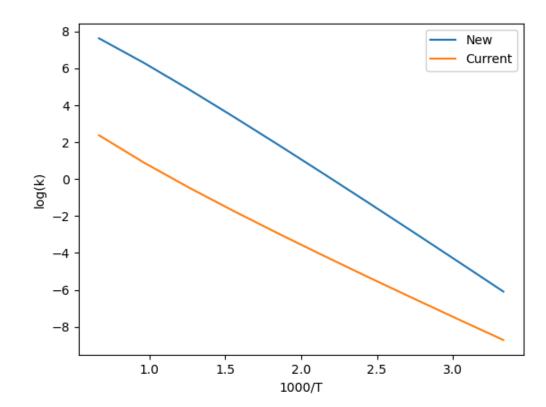
 $\label{eq:analytical_armonius_bm} Arrhenius_{M}(A=(0.00504,\text{'m}^3/(\text{mol*s})'), n=2.41, w0=(301,\text{'kJ/mol'}), E0=(57.3723,\text{'kJ/mol'}), Tmin=(300,\text{'K'}), Tmax=(2000,\text{'K'}), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_N-Sp-5R!H=4R!H_Sp-2R!H=1R!H_Ext-4R!H-R_2R!H->C',), comment=""Estimated from node Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_N-Sp-5R!H=4R!H_Sp-2R!H=1R!H_Ext-4R!H-R_2R!H->C Multiplied by reaction path degeneracy 2.0""")$ 



Arrhenius(A=(1.02e+19,'s^-1'), n=-2.37, Ea=(26400,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

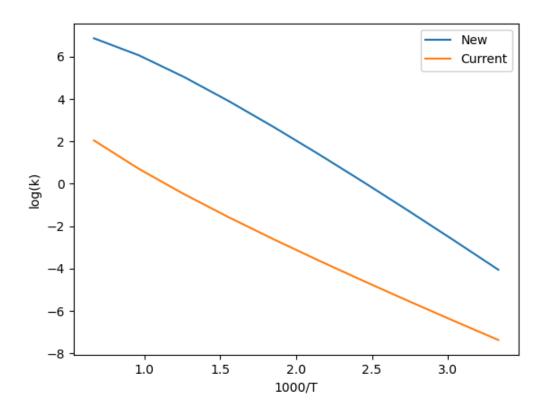
ArrheniusBM(A=(9.07578e-06,'m^3/(mol\*s)'), n=3.04336, w0= (299.503,'kJ/mol'), E0=(64.4187,'kJ/mol'), Tmin=(300,'K'), Tmax= (2000,'K'), uncertainty=RateUncertainty(mu=-0.3757377757886876, var=2.242054186761003, Tref=1000.0, N=1042, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R',), comment="""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R""")



Arrhenius(A=(2.65e+26,'s^-1'), n=-5.02, Ea=(24770,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

 $\label{eq:analytical_constraint} Arrhenius BM(A=(2.06973e-08,'m^3/(mol^*s)'), n=3.60774, w0=(299.574,'kJ/mol'), E0=(49.539,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.5239778944948545, var=2.087050032983542, Tref=1000.0, N=387, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_Ext-3R-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_Ext-4R!H-R_E$ 



Arrhenius(A=(2.83e+26,'s^-1'), n=-5.06, Ea=(26160,'cal/mol'), T0=(1,'K'))

# **Current Kinetics**

 $\label{eq:approx} Arrhenius BM(A=(2.06973e-08,'m^3/(mol^*s)'), n=3.60774, w0=(299.574,'kJ/mol'), E0=(49.539,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.5239778944948545, var=2.087050032983542, Tref=1000.0, N=387, data_mean=0.0, correlation='Root_N-3R-inRing_Ext-3R-R_Ext-4R!H-R_Ext-3R-R_Ext-3R-R_Ext-4R!H-R_Ext-4R!H-R_E$ 

