index: 28  $0 + F \rightarrow co + F$ 

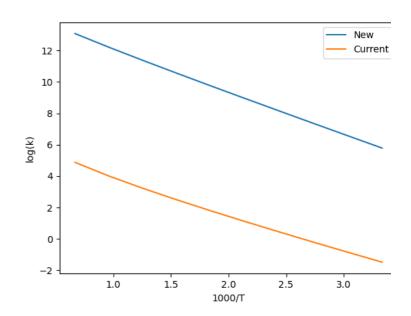
Note: Training reaction written in opposite direction from reaction family.

#### **New Kinetics:**

Arrhenius( $A=(1.78e+12,'s^-1')$ , n=0.79, Ea=(11561.1,'cal/mol'), T0=(1,'K'))

#### **Current Kinetics**

ArrheniusBM(A=(0.329931,'m^3/(mol\*s)'), n=2.07304, w0=(309.5,'kJ/mol'), E0=(35.2326,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.17748312369238067, var=0.6615994821919932, Tref=1000.0, N=9, data\_mean=0.0, correlation='Root\_N-3R->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C',), comment="""Estimated from node Root\_N-3R->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C""")



index: 36  $0 \rightarrow co + F \rightarrow 0$ 

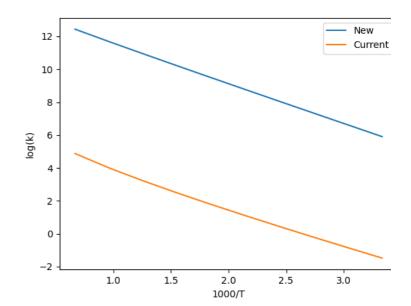
Note: Training reaction written in opposite direction from reaction family.

# **New Kinetics:**

Arrhenius(A= $(5.81e+12, s^-1')$ , n=0.39, Ea=(10740.6, cal/mol'), T0=(1, K'))

# **Current Kinetics**

ArrheniusBM(A=(0.329931,'m^3/(mol\*s)'), n=2.07304, w0=(309.5,'kJ/mol'), E0=(35.2326,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.17748312369238067, var=0.6615994821919932, Tref=1000.0, N=9, data\_mean=0.0, correlation='Root\_N-3R->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C',), comment="""Estimated from node Root\_N-3R->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C""")



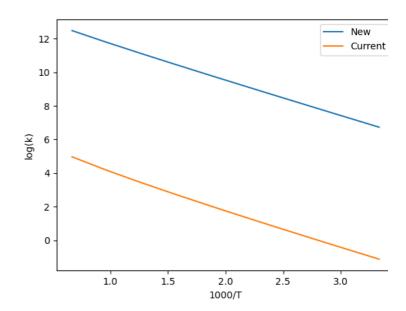
index: 63  $^{\circ}$   $\rightarrow$  co +  $^{\circ}$ 

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

# **New Kinetics:**

#### **Current Kinetics**

ArrheniusBM(A=(86.1,'m^3/(mol\*s)'), n=1.36, w0= (309.5,'kJ/mol'), E0=(36.9208,'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->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C\_Ext-3C-R\_Sp-4R!H-3C\_Ext-3C-R',), comment="""Estimated from node Root\_N-3R->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C\_Ext-3C-R Sp-4R!H-3C\_Ext-3C-R""")



index: 85  $^{\circ}$   $\rightarrow$  co +

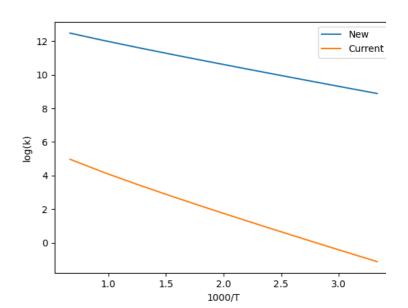
Note: Training reaction written in opposite direction from reaction family.

### **New Kinetics:**

Arrhenius( $A=(3.18e+11, s^-1'), n=0.56, Ea=(5496.44, cal/mol'), T0=(1, K')$ 

# **Current Kinetics**

ArrheniusBM(A=(86.1,'m^3/(mol\*s)'), n=1.36, w0= (309.5,'kJ/mol'), E0=(36.9208,'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->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C\_Ext-3C-R\_Sp-4R!H-3C\_Ext-3C-R',), comment="""Estimated from node Root\_N-3R->O\_N-3BrCCIFHINPSSi-inRing\_3BrCCIFHINPSSi->C\_Ext-3C-R\_Sp-4R!H-3C\_Ext-3C-R\_""")



index:

 $0 + F + F \rightarrow co + F + F$ 

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

# **New Kinetics:**

Arrhenius(A=(2.85e+11,'s^-1'), n=0.68, Ea= (8179.35,'cal/mol'), T0=(1,'K'))

#### **Current Kinetics**

 $\label{eq:arrheniusBM} $$A=(86.1,'m^3/(mol*s)'), n=1.36, w0=(309.5,'k]/mol'), E0=(36.9208,'k]/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->O_N-3BrCCIFHINPSSi-inRing_3BrCCIFHINPSSi->C_Ext-3C-R_Sp-4R!H-3C_Ext-3C-R',), comment="""Estimated from node Root_N-3R->O_N-3BrCCIFHINPSSi-inRing_3BrCCIFHINPSSi->C_Ext-3C-R_Sp-4R!H-3C_Ext-3C-R_""")$ 

