index: 1 $F \stackrel{F}{\longleftarrow} F \rightarrow H \cdot + \stackrel{F}{\longleftarrow}$

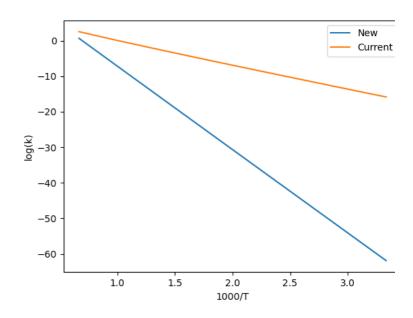
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.53e+15, s^{-1}), n=0.33, Ea=(106892, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(4.1766,'m^3/(mol*s)'), n=1.94174, w0= (205.5,'kJ/mol'), E0=(122.15,'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_1R->H_N-2R->S_N-2BrCCIFHNO-inRing_N-2BrCCIFHNO->O_N-2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_N-4R!H->C_Ext-2C-R',), comment="""Estimated from node Root_1R->H_N-2R->S_N-2BrCCIFHNO-inRing_N-2BrCCIFHNO->O_N-2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_N-4R!H->C_Ext-2C-R""")



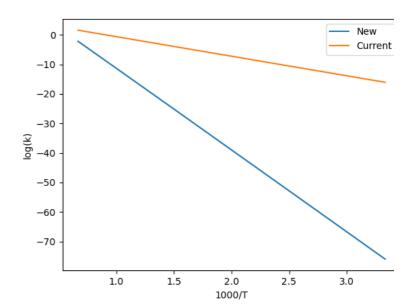
index: 2 $\stackrel{\mathsf{F}}{\swarrow}^{\mathsf{F}} \rightarrow \stackrel{\mathsf{F}}{\searrow}^{\mathsf{F}} + \mathsf{F}$

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

New Kinetics:

Arrhenius($A=(2e+18, 's^-1'), n=-0.61, Ea=(127285, 'cal/mol'), T0=(1, 'K')$)

Current Kinetics

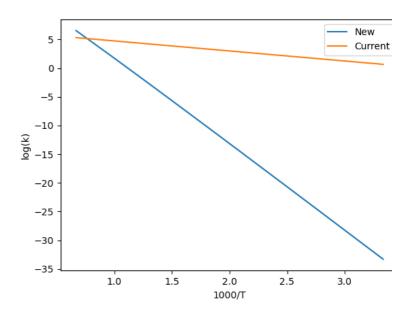


Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Current Kinetics

ArrheniusBM(A=(3.01e+06,'m^3/(mol*s)'), n=-1.3397e-08, w0=(179,'k]/mol'), E0=(33.4345,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Sp-4R!H-2C_Ext-2C-R_N-5R!H->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Sp-4R!H-2C_Ext-2C-R_N-5R!H->C Multiplied by reaction path degeneracy 2.0""")



index: 16 $\stackrel{F}{\underset{F}{\longrightarrow}} \stackrel{F}{\underset{F}{\longrightarrow}} F \rightarrow \stackrel{F}{\underset{F}{\longrightarrow}} F + \stackrel{F}{\underset{F}{\longrightarrow}} F$

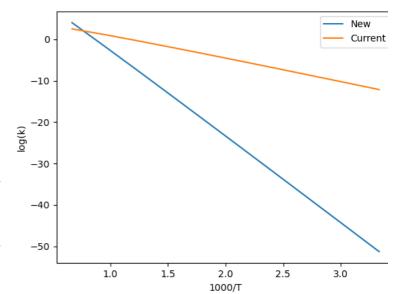
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(9.12e+24, s^-1')$, n=-2.12, Ea=(97427.8, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(2.83587e+13,'m^3/(mol*s)'), n=-2.16473, w0=(173,'k]/mol'), E0=(116.106,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_N-4R!H->O_4BrCCIF->F_Ext-1C-R_N-5R!H->CI_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_N-4R!H->O_4BrCCIF->F_Ext-1C-R_N-5R!H->CI_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R_N-5R!H->CI_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R""")



index: 18 $F \xrightarrow{F} H F \rightarrow H + F \xrightarrow{F} F$

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

New Kinetics:

Arrhenius($A=(3.05e+14, s^-1'), n=0.42, Ea=(103655, cal/mol'), T0=(1, K')$)

Current Kinetics

 $\label{eq:arrheniusBM} $$ A=(1.21692e+34,'m^3/(mol^*s)'), n=-8.80473, w0=(205.5,'k]/mol'), E0=(123.739,'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_1R->H_N-2R->S_N-2BrCCIFHNO-inRing_N-2BrCCIFHNO->O_N-2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->CI_N-5BrCFINOPSSi->Br_N-5CF->C_Sp-4C-2C_Ext-4C-R_Ext-2C-R_Ext-4C-R',), comment="""Estimated from node Root_1R->H_N-2R->S_N-2BrCCIFHNO-inRing_N-2BrCCIFHNO->O_N-2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->CI_N-$

0 - New — Current

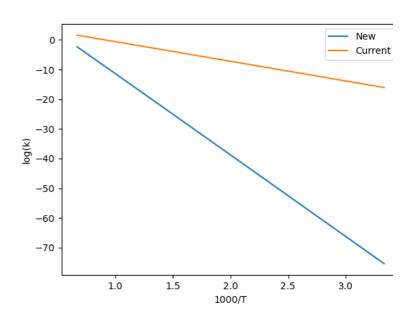
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.91e+18, s^-1')$, n=-0.71, Ea=(126135, 'cal/mol'), T0=(1, K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$ A=(1e+06,'m^3/(mol^*s)'), n=0, w0=(242.5,'k]/mol'), E0=(126.651,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")$



index: 20
$$F \stackrel{F}{\underset{F}{\longrightarrow}} F \rightarrow F \stackrel{F}{\underset{F}{\longrightarrow}} F + F \stackrel{F}{\underset{F}{\longrightarrow}} F$$

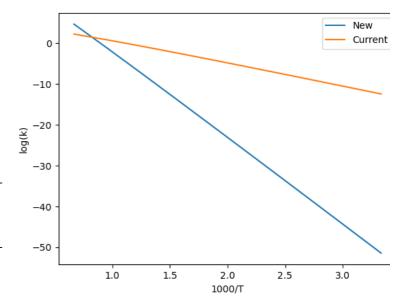
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(3.58e+26, s^{-1}), n=-2.35, Ea=(99025.1, cal/mol'), T0=(1, K'))$

Current Kinetics

ArrheniusBM(A=(1.41794e+13,'m^3/(mol*s)'), n=-2.16473, w0=(173,'k]/mol'), E0=(116.106,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R_N-5R!H->CI_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R_N, comment=""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_N-4R!H->O_4BrCCIF->F_Ext-1C-R_N-5R!H->CI_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R_N-5R!H->CI_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R_""")



index: 21
$$F \xrightarrow{F} F \rightarrow F \xrightarrow{F} F + F$$

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

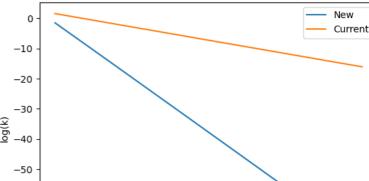
New Kinetics:

Arrhenius($A=(1.57e+19, 's^-1'), n=-0.75, Ea=(125645, 'cal/mol'), T0=(1, 'K')$)

Current Kinetics

ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0= (242.5,'kJ/mol'), E0=(126.651,'kJ/mol'), Tmin=(300,'K'),

 $\label{eq:thmax} Tmax = (2000, 'K'), uncertainty = RateUncertainty (mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")$



index: 29 \rightarrow \rightarrow \rightarrow \leftarrow + F·

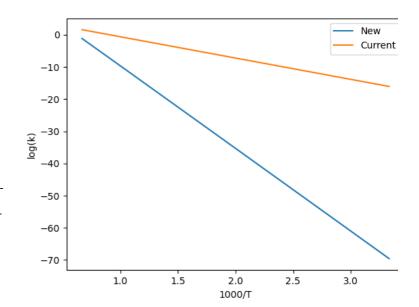
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.78e+17, s^-1')$, n=-0.39, Ea=(117839, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0= (242.5,'k]/mol'), E0=(126.651,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")



index: 30 $\stackrel{\circ}{\triangleright}$ $\stackrel{F}{\longleftarrow}$ $\stackrel{F}{\longrightarrow}$ $\stackrel{\circ}{\longrightarrow}$ + $\stackrel{F}{\longleftarrow}$

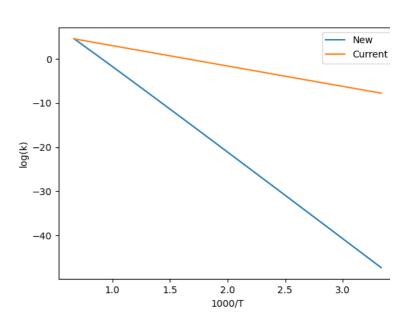
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.79e+23, s^{-1}), n=-1.88, Ea=(91230.4, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment=""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O''")



index: 34 HO
$$+$$
 F \rightarrow F \rightarrow OH + F \leftarrow F

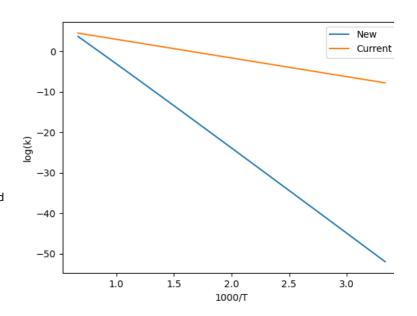
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(2.86e+24,'s^-1')$, n=-2.04, Ea=(98006.3,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment=""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



index: 37 0^{0} F F F O_2

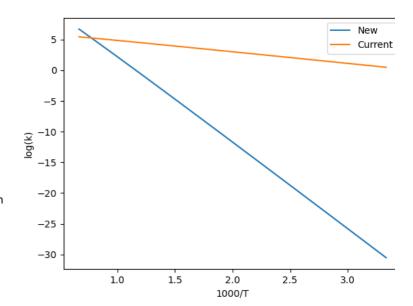
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A= $(3.08e+21,'s^{-1})$, n=-1.64, Ea=(65799.9,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(7.6844e+07,'m^3/(mol*s)'), n=-0.361029, w0=(179,'kJ/mol'), E0=(37.3913,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-1O-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Ext-4R!H-R_Sp-5R!H-4R!H_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-1O-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Ext-4R!H-R_Sp-5R!H-4R!H_Ext-2C-R_Multiplied by reaction path degeneracy 2.0""")



index: 42 $\stackrel{\text{HO}}{\longrightarrow}$ $\stackrel{\text{F}}{\longleftarrow}$ $\stackrel{\text{O}}{\longrightarrow}$ $\stackrel{\text{OH}}{\longrightarrow}$ + $\stackrel{\text{F}}{\longleftarrow}$

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

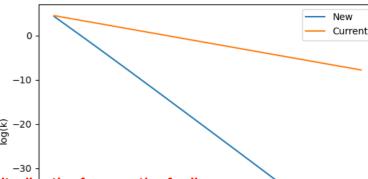
New Kinetics:

Arrhenius(A= $(6.39e+24,'s^-1')$, n=-2.26, Ea=(91093.9,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM($A=(4e+07, m^3/(mol^*s)')$, n=0, w0=(173, kJ/mol'), E0=(88.2769, 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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



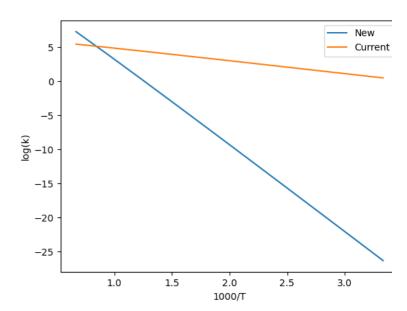
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.03e+21,'s^-1')$, n=-1.6, Ea=(59501.3,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(7.6844e+07,'m^3/(mol*s)'), n=-0.361029, w0=(179,'k]/mol'), E0=(37.3913,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Ext-4R!H-R_Sp-5R!H-4R!H_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Ext-4R!H-R_Sp-5R!H-4R!H_Ext-2C-R_Multiplied by reaction path degeneracy 2.0""")



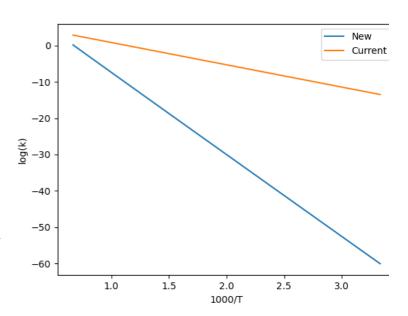
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.67e+13, s^-1'), n=0.61, Ea=(102677, cal/mol'), T0=(1, K')$)

Current Kinetics

 $\label{eq:arrheniusBM} $$ A=(1e+07,'m^3/(mol^*s)'), n=0, w0=(205.5,'k]/mol'), E0=(117.474,'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_1R->H_N-2R->S_N-2BrCCIFHNO-inRing_N-2BrCCIFHNO->O_N-2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->C_N-5BrCFINOPSSi->Br_5CF->C',), comment="""Estimated from node Root_1R->H_N-2R->S_N-2BrCCIFHNO-inRing_N-2BrCCIFHNO->O_N-2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->C_N-5BrCFINOPSSi->Br_5CF->C""")$



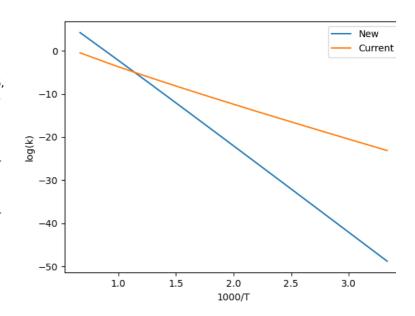
index: 53
$$\stackrel{F}{\rightleftharpoons} \stackrel{F}{\rightleftharpoons} \stackrel{$$

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

Arrhenius($A=(8.35e+23,'s^{-1})$), n=-1.92, Ea=(93296.2,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 54 $\stackrel{F}{\rightleftharpoons}$ $\stackrel{F}{\rightleftharpoons}$ $\stackrel{F}{\rightleftharpoons}$ $\stackrel{F}{\rightleftharpoons}$ $\stackrel{F}{\rightleftharpoons}$ $\stackrel{F}{\rightleftharpoons}$

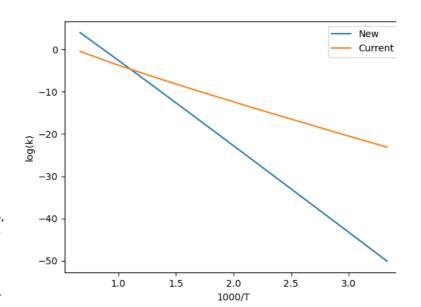
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(4e+24,'s^-1'), n=-2.11, Ea=(95383.9,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



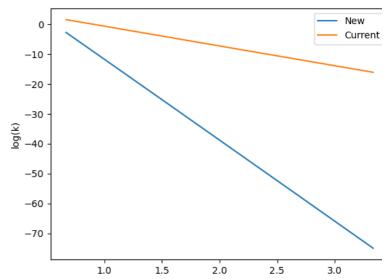
index: 55 $\stackrel{\mathsf{F}}{\triangleright} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}}{\vdash} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{\mathsf{F}} \stackrel{$

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

Arrhenius($A=(1.19e+17, s^-1'), n=-0.52, Ea=(124543, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0= (242.5,'k]/mol'), E0=(126.651,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C'"")



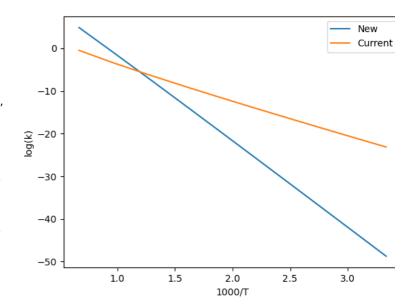
Note: Training reaction written in opposite direction from reaction family.07

New Kinetics:

Arrhenius($A=(1.21e+25, s^{-1}), n=-2.03, Ea=(94408.1, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 58 F $\stackrel{F}{=}$ F $\stackrel{F}{=}$ F $\stackrel{F}{=}$ F + F.

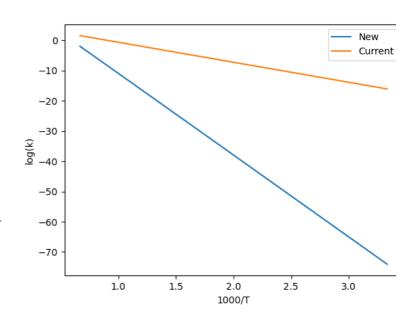
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(3.16e+17, s^{-1}), n=-0.43, Ea=(124181, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0= (242.5,'kJ/mol'), E0=(126.651,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")



index: 64
$$\stackrel{\circ}{\triangleright}$$
 $\stackrel{\circ}{\models}$ $\stackrel{\circ}{\models}$ $\stackrel{\circ}{\triangleright}$ $\stackrel{\circ}{\triangleright}$ $\stackrel{\circ}{\models}$ $\stackrel{\circ}{\triangleright}$

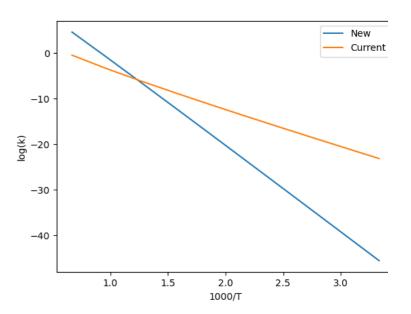
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(5.93e+22,'s^-1'), n=-1.68, Ea=(88047.8,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$ A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")$



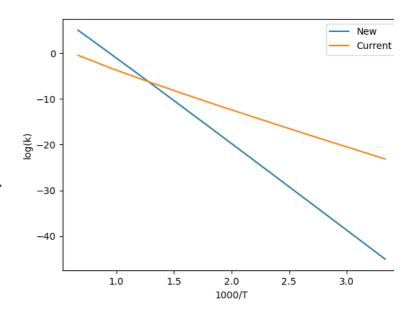
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(3.54e+23,'s^{-1})$), n=-1.79, Ea=(88037,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



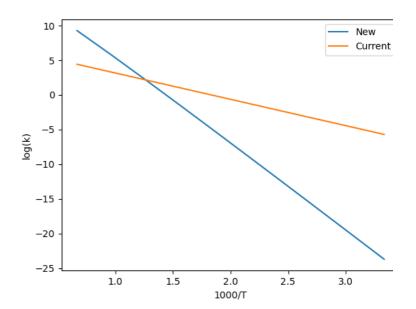
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(4.66e+24,'s^-1'), n=-2.13, Ea=(59169.3,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")



index: 71 $_{F}$ $_{F}$

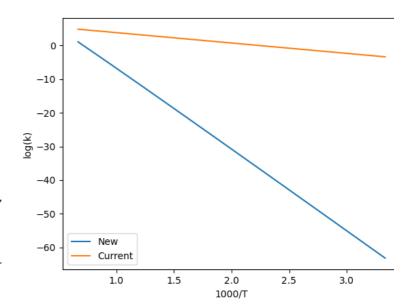
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.96e+23, s^{-1}), n=-2.01, Ea=(112565, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'),
n=1.31229e-07, w0=(179,'k]/mol'), E0=(58.9141,'k]/mol'),
Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=0.016021952005170214, var=0.3543710496450803,
Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C',)



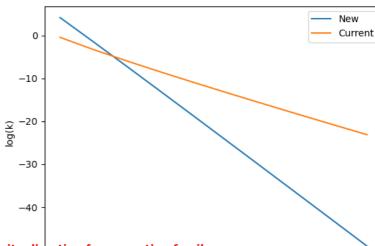
index: 77 $F \xrightarrow{F} F = OH \rightarrow F \rightarrow OH + F \rightarrow F$

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

New Kinetics:

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R'"")



index: 78 F $\stackrel{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}}{\overset{\mathsf{F}}}}}{\overset{\mathsf{F}}{\overset{\mathsf{F}}}}}}{\mathsf{OH}}}}}}}}}} index}$

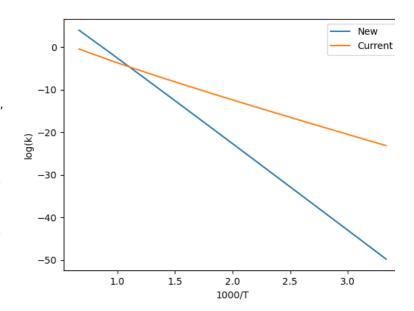
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(2.29e+23,'s^-1')$, n=-1.78, Ea=(94310.4,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 80 $_{F}$ $\stackrel{F}{\longleftarrow}_{F}$ $\stackrel{\bullet}{\longrightarrow}_{F}$ $\stackrel{\bullet}{\longrightarrow}_{F}$ $\stackrel{\bullet}{\longrightarrow}_{F}$ $\stackrel{\bullet}{\longrightarrow}_{F}$

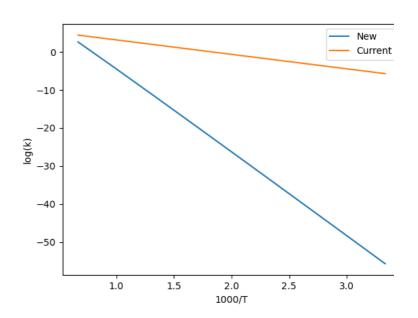
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(7.69e+23,'s^{-1}), n=-2, Ea=(102396,'cal/mol'), T0=(1,'K')$)

Current Kinetics

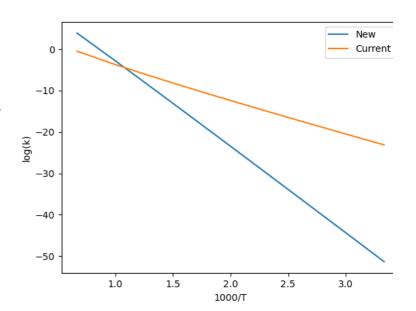
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'k]/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")



Arrhenius($A=(5.87e+24,'s^--1')$, n=-2.1, Ea=(97369.7,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



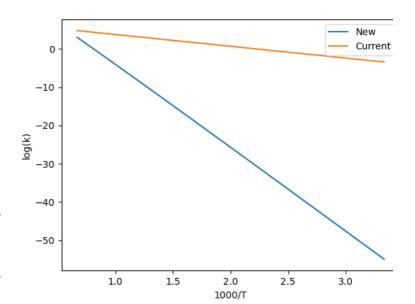
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(4.51e+23, s^{-1}), n=-1.81, Ea=(101746, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.016021952005170214, var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C'""")

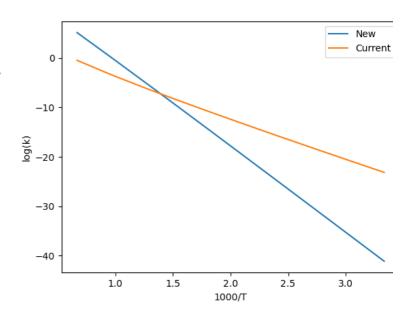


Note: Training reaction written in opposite direction from reaction family.

Arrhenius(A= $(7.01e+21, s^-1')$, n=-1.53, Ea=(81204.1, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 92 $\stackrel{\circ}{\longrightarrow}_{F}$ \rightarrow $\stackrel{\circ}{\longrightarrow}_{F}$ $\stackrel{\circ}{\longrightarrow}_{F}$

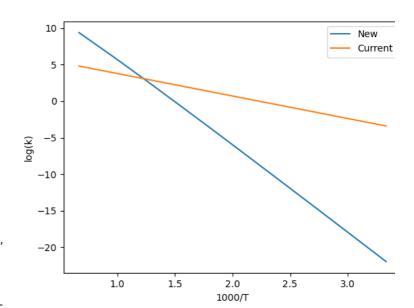
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(4.57e+25,'s^-1'), n=-2.52, Ea= (56793.8,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.016021952005170214, var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C'""")



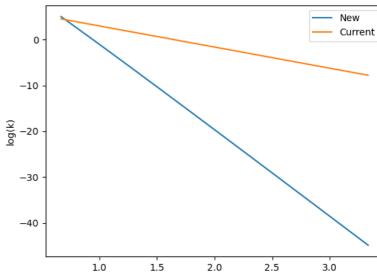
index: 97 $\stackrel{\text{HO}}{\longrightarrow}$ $\stackrel{\text{F}}{\longrightarrow}$ $\stackrel{\text{F$

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

Arrhenius(A=(1.61e+24,'s^-1'), n=-2, Ea=(88017.7,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'k)/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



index: 98 \xrightarrow{HO} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}

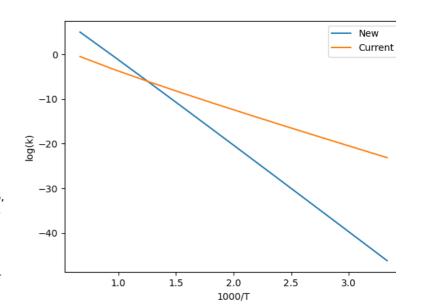
Note: Training reaction written in opposite direction from reaction family വാ

New Kinetics:

Arrhenius($A=(7.54e+24,'s^--1')$, n=-2.1, Ea=(90470.1,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, $$w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")$



index:

 $F \downarrow 0 \downarrow F \rightarrow F \downarrow 0 \downarrow 0 + F \downarrow 0$

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

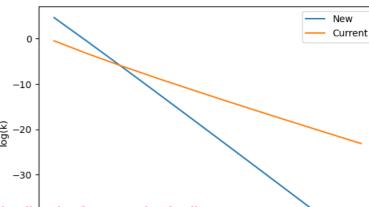
New Kinetics:

Arrhenius(A=(1.4e+25,'s^-1'), n=-2.35, Ea=(89361.9,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246,

w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index:

 $F \downarrow 0 \downarrow F \rightarrow 0 \downarrow F + F \downarrow 0$

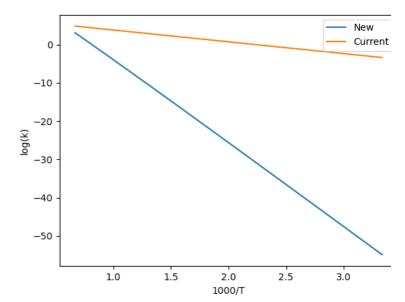
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.96e+24, s^-1'), n=-2.17, Ea=(102065, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'),
n=1.31229e-07, w0=(179,'k]/mol'), E0=(58.9141,'k]/mol'),
Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=0.016021952005170214, var=0.3543710496450803,
Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C'"")



index: 105

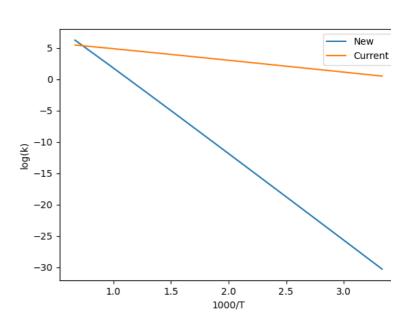
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(5.31e+19, s^{-1}), n=-1.31, Ea=(64218.7, cal/mol'), T0=(1, K')$)

Current Kinetics

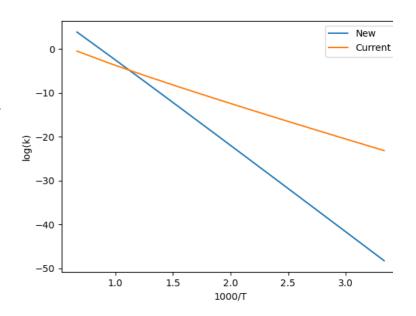
ArrheniusBM(A=(7.6844e+07,'m^3/(mol*s)'), n=-0.361029, w0=(179,'k]/mol'), E0=(37.3913,'k]/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-10-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Ext-4R!H-R_Sp-5R!H-4R!H_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-10-R_3R!H->O_2R->C_N-2C-inRing_Ext-2C-R_Ext-4R!H-R_Sp-5R!H-4R!H_Ext-2C-R_Multiplied by reaction path degeneracy 2.0""")



Arrhenius(A= $(5.01e+22, s^-1')$, n=-1.73, Ea=(91468.2, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 112

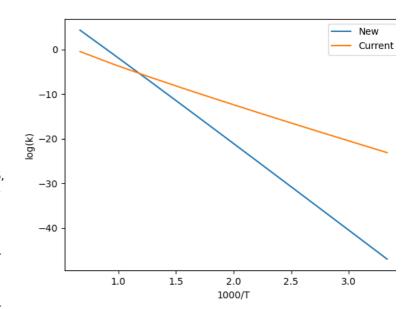
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(4.02e+23, s^-1'), n=-1.92, Ea=(90402.8, cal/mol'), T0=(1, 'K'))$

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->C_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index:

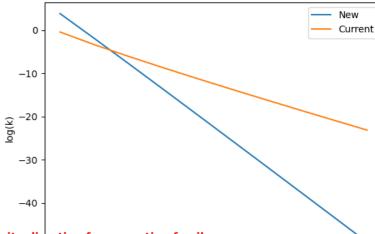
$$\begin{bmatrix} F & F & F & F \\ F & F & F \end{bmatrix} \rightarrow \begin{bmatrix} F & F & F \\ F & F & F \end{bmatrix} + \begin{bmatrix} F & F & F \\ F & F & F \end{bmatrix}$$

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

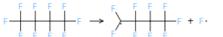
New Kinetics:

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R'"")



index:



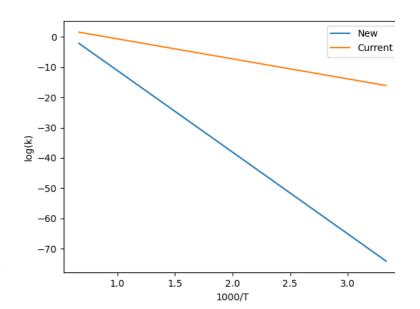
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(4.58e+16, s^{-1}), n=-0.24, Ea=(123786, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0= (242.5,'kJ/mol'), E0=(126.651,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C_""")



index: F F F F -

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

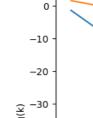
New Kinetics:

Arrhenius($A=(1.5e+16, s^{-1}), n=-0.25, Ea=(115077, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0= (242.5,'kJ/mol'), E0=(126.651,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1B

1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")



index:

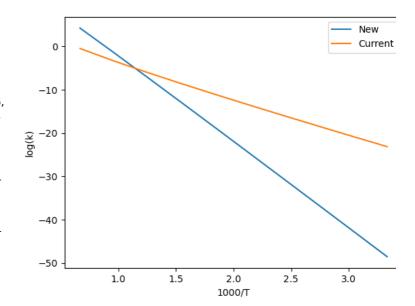
Note: Training reaction written in opposee direction from reaction family

New Kinetics:

Arrhenius($A=(4.06e+23, s^{-1}), n=-1.84, Ea=(92772.2, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



Current

index: 118

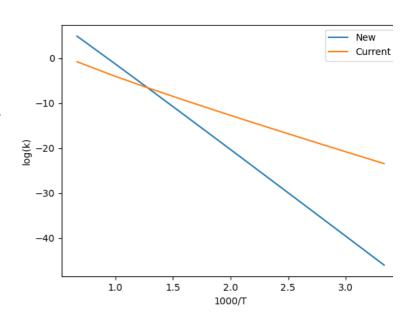
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.8e+23,'s^{-1})$), n=-1.84, Ea=(89619.2,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$A=(1.31566e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")$



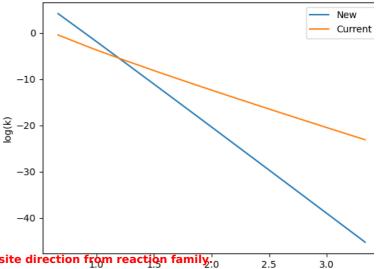
index:

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

New Kinetics:

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R'"")



index: 123

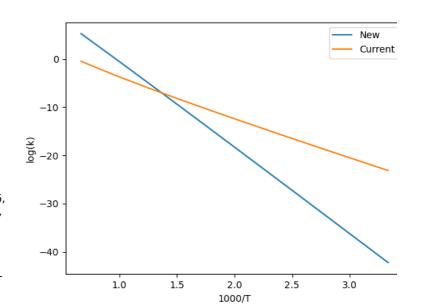
Note: Training reaction written in opposite direction from reaction family:

New Kinetics:

Arrhenius($A=(2.42e+22, s^-1'), n=-1.56, Ea=(83413.6, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R'"")



index:

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

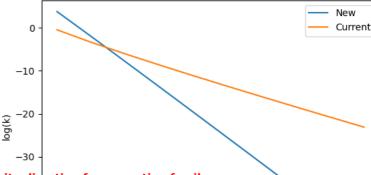
New Kinetics:

Arrhenius(A=(2.09e+22,'s^-1'), n=-1.56, Ea=(93214.4,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$A$=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, $$w0=(173,'kJ/mol'), E0=(139.101,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, molecular contents), and the second contents of the second contents o$

var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 128

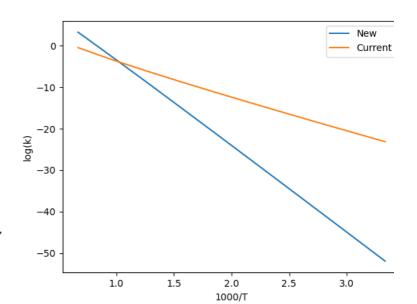
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A= $(3.69e+24,'s^-1')$, n=-2.24, Ea=(97357.9,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, $$w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->0_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->0_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")$



index: 129 $F \xrightarrow{F} 0 \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F$

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

New Kinetics:

Arrhenius($A=(2.17e+24, s^-1')$, n=-2.17, Ea=(55469.8, 'cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A= $(9.04e+06, 'm^3/(mol*s)')$, n=2.17087e-08, w0=(179, 'k]/mol'), E0=(72.7054, '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-1R->H N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), 10 comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R_N-3R!H->0_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""") 5 0 -5 log(k)

index: 130

-10

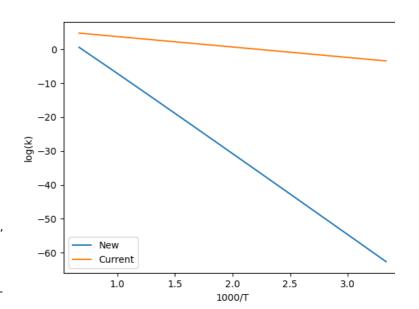
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(1.33e+23,'s^-1'), n=-1.99, Ea= (111007, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM($A=(7.38316e+06, 'm^3/(mol*s)')$, n=1.31229e-07, w0=(179, k]/mol'), E0=(58.9141, k]/mol'), Tmin=(300, 'K'), Tmax=(2000, 'K'),uncertainty=RateUncertainty(mu=-0.016021952005170214, var=0.3543710496450803, Tref=1000.0, N=2, data mean=0.0, correlation='Root N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',), comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C""")



New

Current

index: 137

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

New Kinetics:

Arrhenius(A=(3.66e+22,'s^-1'), n=-1.67, Ea= (91685, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R 3R!H->F Ext-2CF-R Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-

1BrcCIFINOPSSi->N_N-1BrcCIFOS->CI_N-1BrcFoS->O_N-1BrcFS-inRing_1BrcFS->C_N-2R->S_N-2BrcF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R"")

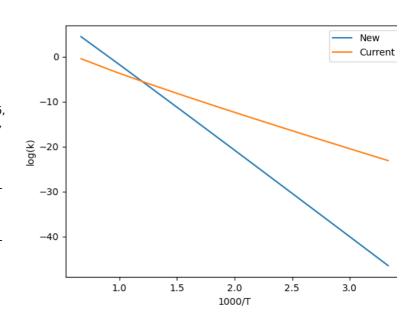


New Kinetics:

Arrhenius(A=(5.6e+22,'s^-1'), n=-1.66, Ea= (89416.2,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



New Current

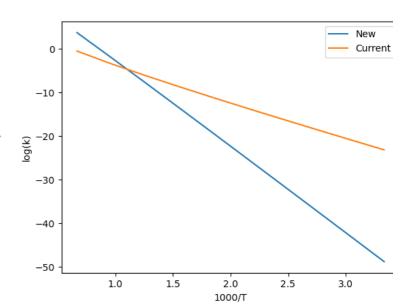
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A= $(3.16e+22, s^-1')$, n=-1.67, Ea=(92160.7, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



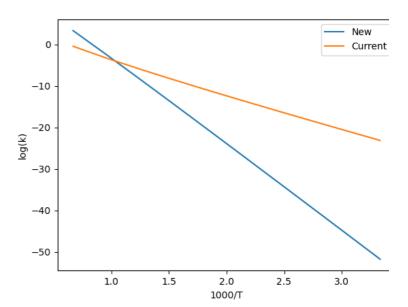
index: 141 $F \stackrel{F}{\longleftarrow} F \stackrel{F}{\longrightarrow} F \rightarrow F \stackrel{F}{\longrightarrow} F \stackrel{F}{\longleftarrow} F \stackrel{F}{\longleftarrow} F \stackrel{F}{\longrightarrow} F \stackrel{\longrightarrow} F \stackrel{F}{\longrightarrow} F \stackrel{F}{\longrightarrow} F \stackrel{F}{\longrightarrow} F \stackrel{F}{\longrightarrow} F \stackrel{F}{\longrightarrow} F \stackrel{F}{\longrightarrow} F$

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

Arrhenius($A=(2.29e+25, s^-1')$, n=-2.47, Ea=(97424.5, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 142

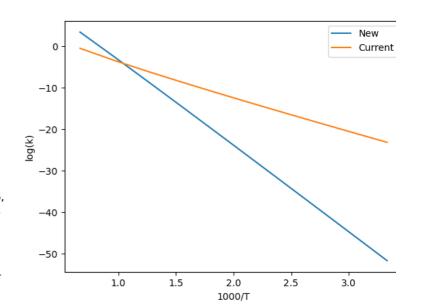
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(4.69e+24,'s^-1')$, n=-2.22, Ea=(97230.6,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index: 143

 $F \xrightarrow{F} \xrightarrow{O} \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F$

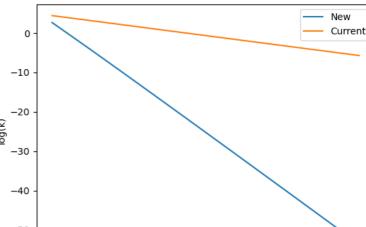
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.76e+23,'s^{-1})$), n=-2.12, Ea=(99032,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$A=(9.04e+06,'m^3/(mol^*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R_""")$



index:

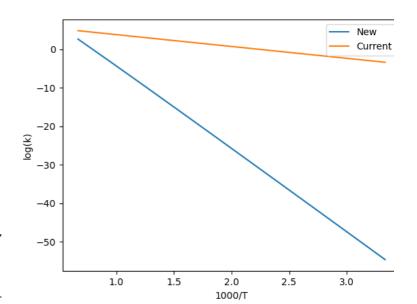
Note: Training reaction written in opposite threction from reaction family.

New Kinetics:

Arrhenius($A=(1.63e+23, s^-1'), n=-1.87, Ea=(100523, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'),
n=1.31229e-07, w0=(179,'k]/mol'), E0=(58.9141,'k]/mol'),
Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=0.016021952005170214, var=0.3543710496450803,
Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C'""")



index: 147 0 F F F → F F 0 + F ✓ 0

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

New Kinetics:

Arrhenius($A=(3.61e+20, 's^-1'), n=-1.3, Ea=(86978.3, 'cal/mol'), T0=(1, 'K')$)

Current Kinetics

 $\label{eq:arrheniusBM} $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), Tmin=(300,'K'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), Tmin=(300,'K'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), Tmin=(300,'K'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'mol*s), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'mol*s), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'model), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'model), uncertainty=RateUncertainty(mu=0.0, model) $$ArrheniusBM(A=(2.63131e-11,'model), uncertainty=RateUncertainty$

var=33.13686319048999, Tref=1000.0, N=1, data_mean=0.0, correlation='Root_N-1R->H N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C- $R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',),$ comment="""Estimated from node Root N-1R->H N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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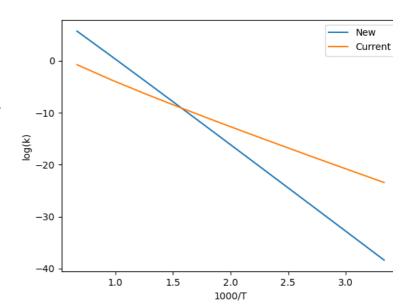
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(2.49e+21,'s^-1'), n=-1.4, Ea= (77266.7, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(1.31566e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173, k]/mol'), E0=(139.101, 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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C- $R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',),$ comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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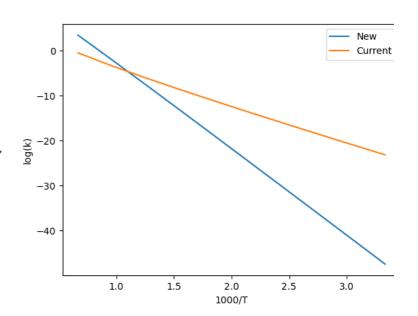
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(9.11e+21,'s^-1'), n=-1.72, Ea= (89384.1, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R 3R!H->F Ext-2CF-R Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



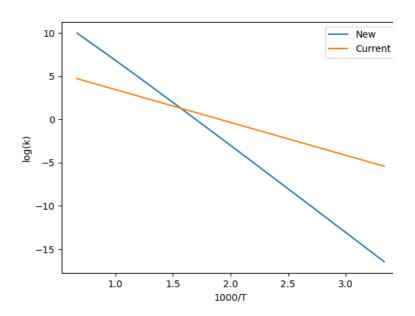
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(3.2e+22,'s^-1'), n=-1.76, Ea=(47485.2,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(1.808e+07,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R_Multiplied by reaction path degeneracy 2.0""")



index:

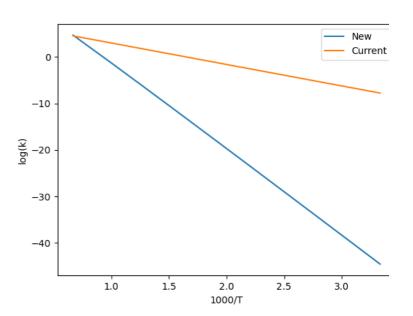
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.5e+23,'s^{-1})$, n=-1.85, Ea=(86653.7,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'k]/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-2CF-R_4R!H->F_Ext-2CF-R_4R!H->O""")



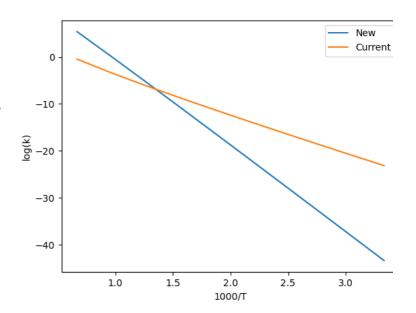
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(1.18e+24,'s^-1'), n=-1.94, Ea= (85953.1, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173, k]/mol'), E0=(139.101, 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-1R->H N 1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R $3R!H->F_Ext-2CF-R_Ext-4R!H-R',),$ comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C- $R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")$



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$$\begin{array}{c|c} \mathsf{HO} & \mathsf{F} & \mathsf{F} & \mathsf{F} \\ \mathsf{O} & \mathsf{E} & \mathsf{E} & \mathsf{E} \end{array} \rightarrow \begin{array}{c|c} \mathsf{HO} & \mathsf{F} & \mathsf{F} \\ \mathsf{O} & \mathsf{E} & \mathsf{F} \end{array} \rightarrow \begin{array}{c|c} \mathsf{F} & \mathsf{F} \\ \mathsf{E} \end{array}$$

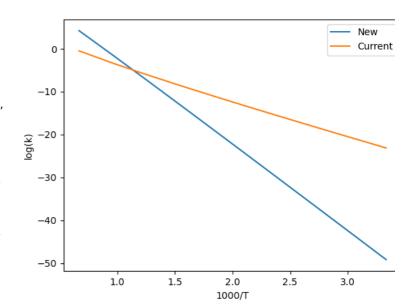
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(1.87e+24,'s^-1'), n=-1.99, Ea= (94065, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173, k]/mol'), E0=(139.101, 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-1R->H N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R 3R!H->F Ext-2CF-R Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R 3R!H->F Ext-2CF-R Ext-4R!H-R""")



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

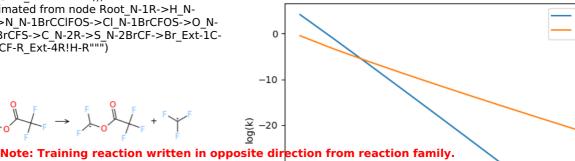
New Kinetics:

Arrhenius($A=(6.61e+24, 's^-1'), n=-2.42, Ea=$ (88881.4, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-

1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C- $R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',),$ comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



Current

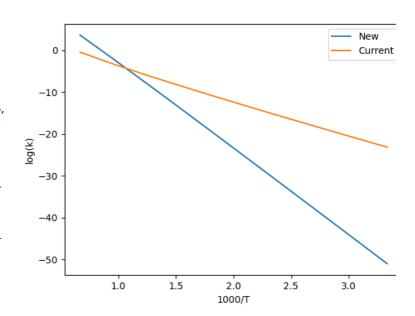
index: 165

New Kinetics:

Arrhenius(A=(6.89e+25,'s^-1'), n=-2.56, Ea= (96716.7, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R 3R!H->F Ext-2CF-R Ext-4R!H-R',), comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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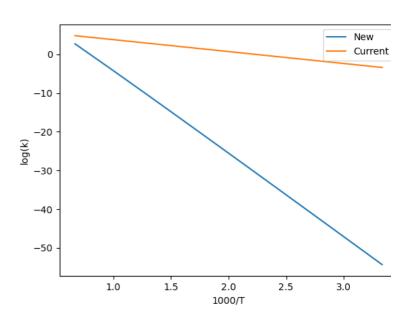
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(1.78e+24,'s^-1'), n=-2.18, Ea= (100406, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM($A=(7.38316e+06, 'm^3/(mol*s)')$, n=1.31229e-07, w0=(179, kJ/mol'), E0=(58.9141, kJ/mol'), Tmin=(300, 'K'), Tmax=(2000, 'K'),uncertainty=RateUncertainty(mu=-0.016021952005170214, var=0.3543710496450803, Tref=1000.0, N=2, data mean=0.0, correlation='Root N-1R->H N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R N-3R!H->O Ext-2R-R 2R->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C""")



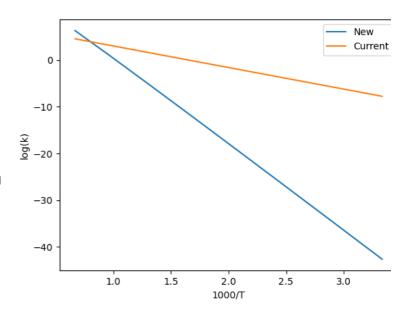
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Note: Training reaction written in opposite direction from reaction family.

Arrhenius(A= $(3.23e+25, s^{-1})$, n=-2.09, Ea=(86406.5, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



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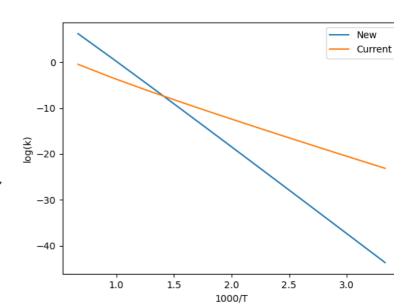
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.18e+26, s^-1'), n=-2.2, Ea=(88258.3, cal/mol'), T0=(1, K')$

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R'"")



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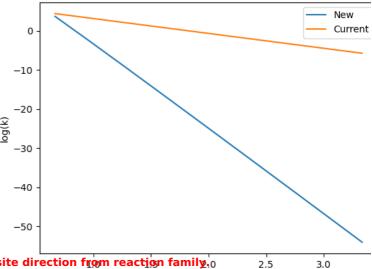
$$F \xrightarrow{\downarrow 0} F \xrightarrow{\downarrow 0} F$$

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

New Kinetics:

Current Kinetics

ArrheniusBM(A=(9.04e+06, 'm^3/(mol*s)'), n=2.17087e-08, w0=(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R_N-3R!H->0_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")



3.0

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$$F \xrightarrow{\downarrow} F \xrightarrow{\downarrow}$$

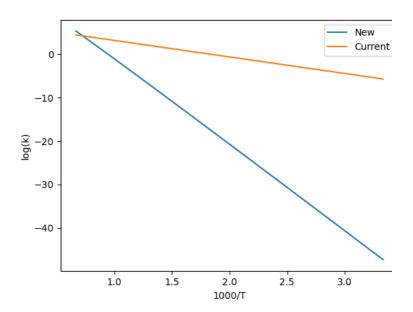
Note: Training reaction written in opposite direction from reaction family.0

New Kinetics:

Arrhenius(A=(2.66e+25,'s^-1'), n=-2.08, Ea= (92732.9, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM($A=(9.04e+06, 'm^3/(mol*s)'), n=2.17087e-$ 08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl 1BrCFOS->O Ext-10-R_N-3R!H->0_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-10-R N-3R!H->O Ext-2R-R 2R->C Ext-2C-R Ext-2C-R""")



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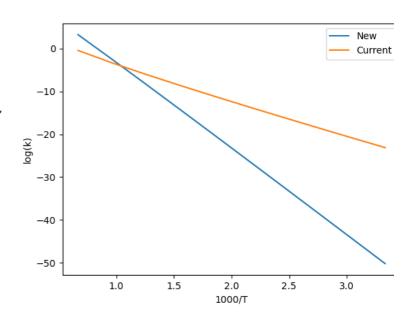
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(4.03e+23,'s^-1'), n=-2.1, Ea= (94143.9, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11, 'm^3/(mol*s)'), n=4.71246, w0=(173, k]/mol'), E0=(139.101, 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-1R->H N-1BrCClFINOPSSi->N N-1BrCClFOS->Cl N-1BrCFOS->O N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R 3R!H->F Ext-2CF-R Ext-4R!H-R',)comment="""Estimated from node Root N-1R->H N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing 1BrCFS->C N-2R->S N-2BrCF->Br Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



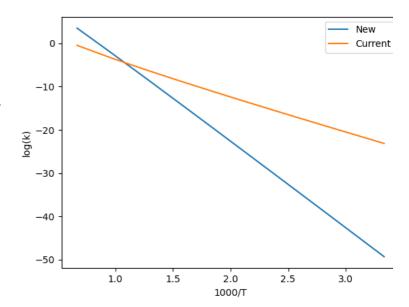
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.39e+23, 's^-1')$, n=-2.11, Ea=(93175.6, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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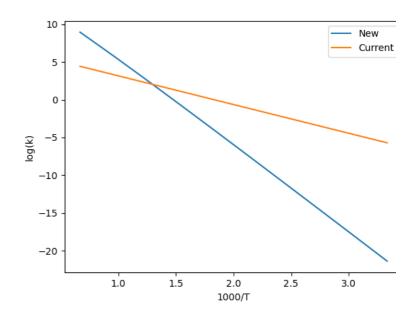
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(2.25e+23,'s^{-1})$), n=-2.04, Ea=(54440.6,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R'"")



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$$F \xrightarrow{F} F \xrightarrow{F} O \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} O$$

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

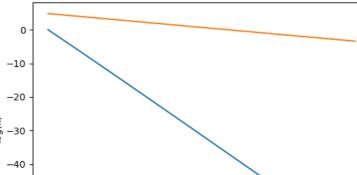
New Kinetics:

Arrhenius(A= $(1.19e+22, 's^--1')$, n=-1.86, Ea=(110777, 'cal/mol'), T0=(1, 'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$A$=(7.38316e+06,'m^3/(mol*s)'), $$n=1.31229e-07, $w0=(179,'kJ/mol'), $E0=(58.9141,'kJ/mol'), $$$

$$\begin{split} & Tmin = (300, \text{'K'}), \ Tmax = (2000, \text{'K'}), \\ & uncertainty = RateUncertainty(mu = 0.016021952005170214, \ var = 0.3543710496450803, \\ & Tref = 1000.0, \ N = 2, \ data_mean = 0.0, \ correlation = \text{'Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C',), \\ & comment = \text{"""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C""") \end{split}$$



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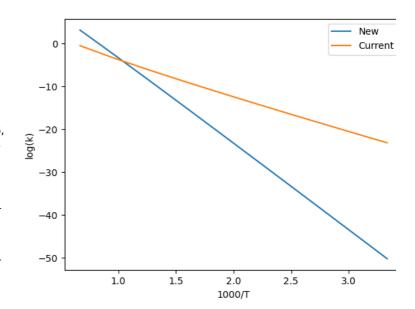
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(8.64e+23,'s^{-1}), n=-2.21, Ea=(94232.2,'cal/mol'), T0=(1,'K'))$

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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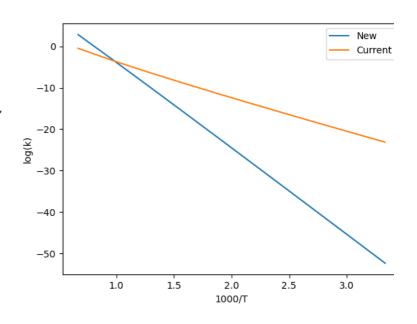
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A= $(1.95e+23,'s^{-1})$), n=-1.98, Ea=(97110.9,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



index:

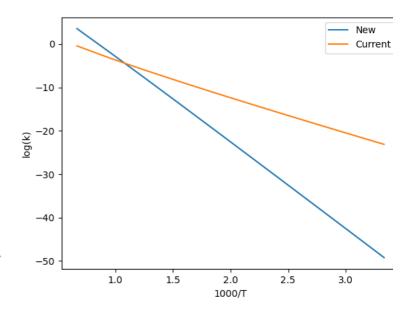
Note: Training reaction written in opposite direction from reaction family.



Arrhenius(A= $(1.47e+24,'s^-1')$, n=-2.23, Ea=(93133.7,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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

New Kinetics:

Arrhenius(A= $(2.58e+22,'s^{-1})$), n=-1.88, Ea=(97794.3,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(9.04e+06, 'm^3/(mol*s)'), n=2.17087e-08, w0=(179, 'k]/mol'), E0=(72.7054, '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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")

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

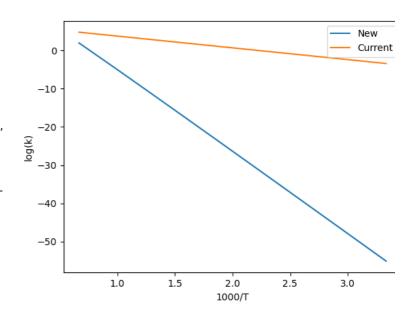
- New - Current

New Kinetics:

Arrhenius($A=(5.38e+21,'s^{-1}), n=-1.63, Ea=(99985,'cal/mol'), T0=(1,'K')$)

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.016021952005170214, var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C""")



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$$\begin{array}{c|c} HO & F & F & F \\ \hline \end{array} \rightarrow \begin{array}{c} HO & F & F \\ \hline \end{array} + \begin{array}{c} F \\ \hline \end{array} + \begin{array}{c} F \\ \hline \end{array}$$

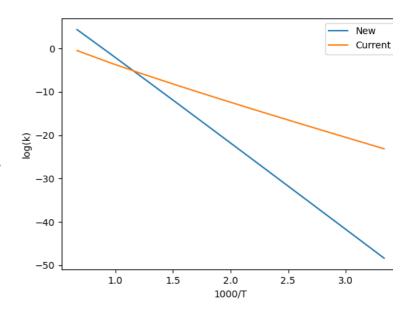
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(6.29e+22, s^{-1}), n=-1.56, Ea=(92402.5, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



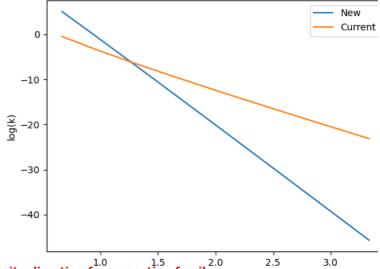
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Note: Training reaction written in opposite direction from reaction family.

Arrhenius(A=(9.56e+22,'s^-1'), n=-1.56, Ea=(88931.2,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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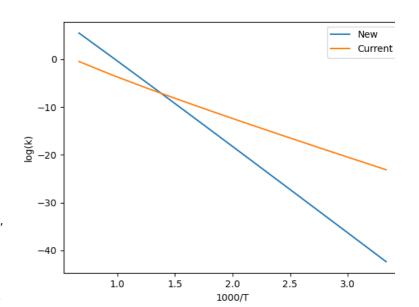
Note: Training reaction written in opposite direction from reaction family 0.0/T

New Kinetics:

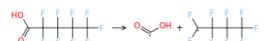
Arrhenius(A=(3.6e+22,'s^-1'), n=-1.52, Ea=(83972.4,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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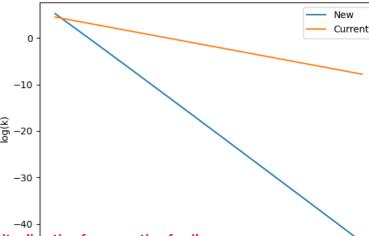
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.98e+22, s^{-1}), n=-1.41, Ea=(86114, cal/mol'), T0=(1, K'))$

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'k]/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



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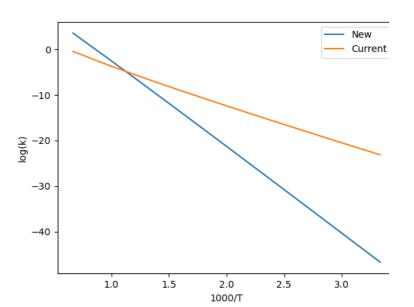
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(2.29e+23,'s^{-1})$), n=-2.17, Ea=(88723.3,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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

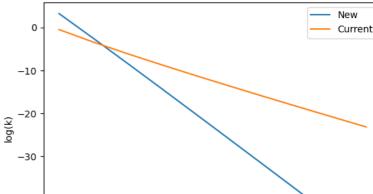
New Kinetics:

Arrhenius($A=(1.72e+24, 's^-1'), n=-2.29, Ea=(94058.5, 'cal/mol'), T0=(1, 'K')$)

Current Kinetics

ArrheniusBM(A= $(2.63131e-11, m^3/(mol^*s)')$, n=4.71246, w0=(173, kJ/mol'), E0=(139.101, 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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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 $\downarrow 0$ $\downarrow F$ $\downarrow 0$ $\downarrow F$ $\downarrow F$ $\downarrow F$

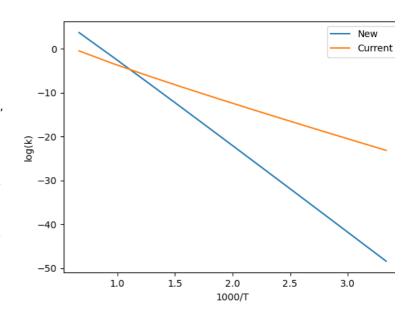
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(3.04e+24,'s^-1')$, n=-2.31, Ea=(92177.2,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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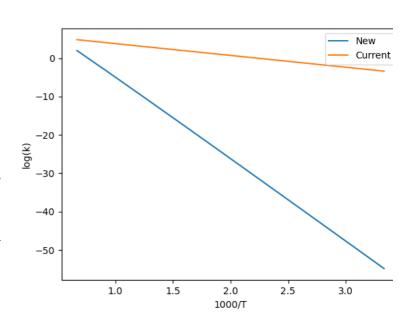
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(4.06e+22, s^{-1}), n=-1.92, Ea=(99819.7, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'),
n=1.31229e-07, w0=(179,'k]/mol'), E0=(58.9141,'k]/mol'),
Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=0.016021952005170214, var=0.3543710496450803,
Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C'"")



 $F \xrightarrow{F} O \xrightarrow{F} F \rightarrow O \xrightarrow{OH} + F \xrightarrow{F} F$

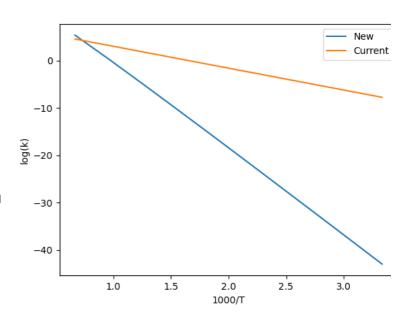
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(4.26e+27, s^{-1}), n=-3.05, Ea=(86516.1, cal/mol'), T0=(1, K')$)

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



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F F O F F O OH + F F

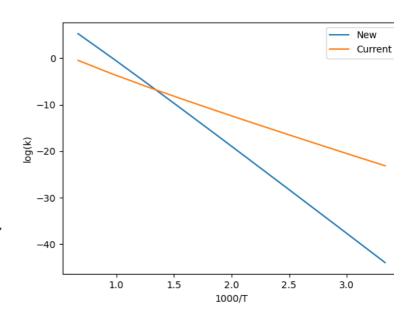
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A= $(1.51e+28, s^-1')$, n=-3.16, Ea=(88261.4, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



 $F \xrightarrow{F} O \xrightarrow{F} F \xrightarrow{F} O \xrightarrow{F} O + F \rightarrow F O$

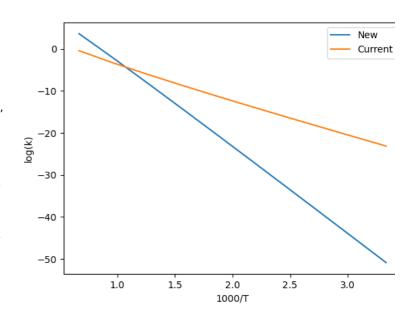
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A= $(8.87e+27,'s^-1')$, n=-3.21, Ea=(97239.1,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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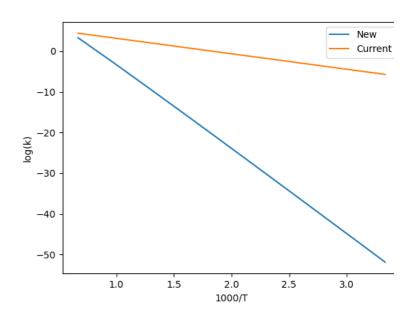
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius(A=(6.3e+26,'s^-1'), n=-2.9, Ea= (98101.1,'cal/mol'), T0=(1,'K'))

Current Kinetics

 $\label{eq:arrheniusBM} $$ A=(9.04e+06,'m^3/(mol^*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")$



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$$F \xrightarrow{F} 0 \xrightarrow{\text{HO}} F \xrightarrow{F} + \cdot 0 \xrightarrow{F} F$$

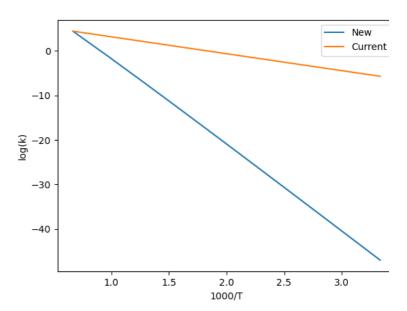
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.57e+27, s^{-1}), n=-2.97, Ea=(91728.9, cal/mol'), T0=(1, 'K'))$

Current Kinetics

ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")



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$$F \xrightarrow{F} F \xrightarrow{O} F \xrightarrow{F} F \xrightarrow{O} OH + F \xrightarrow{F} F \xrightarrow{F} F$$

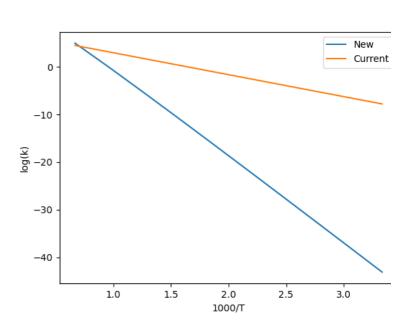
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(5.75e+27,'s^-1'), n=-3.2, Ea=(86426.9,'cal/mol'), T0=(1,'K'))$

Current Kinetics

ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0= (173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")



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$$F \xrightarrow{F} O \xrightarrow{F} F \xrightarrow{OH} F \xrightarrow{F} F \xrightarrow{F} F$$

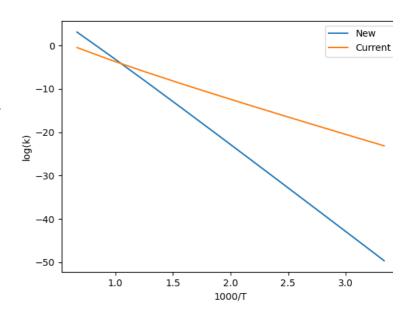
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(3.09e+27,'s^-1')$, n=-3.34, Ea=(94502.6,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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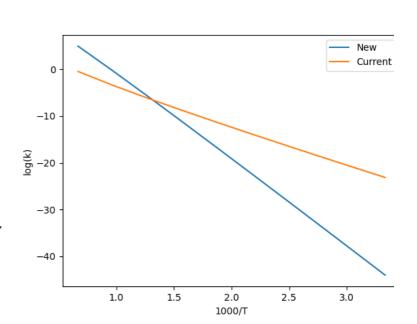
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(2.03e+28, s^{-1}), n=-3.32, Ea=(87974.5, cal/mol'), T0=(1, 'K'))$

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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$$F \xrightarrow{F} OH + F \xrightarrow{$$

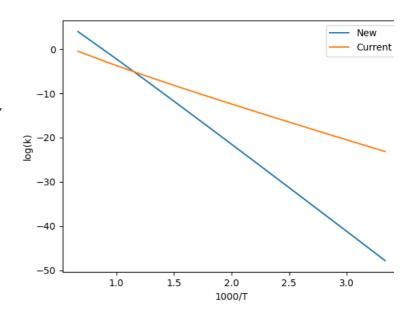
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:

Arrhenius($A=(1.48e+28, s^{-1}), n=-3.36, Ea=(92858.7, cal/mol'), T0=(1, K'))$

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'k]/mol'), E0=(139.101,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->CI_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")



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$$F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{HO} F F + F \xrightarrow{F} F F$$

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

New Kinetics:

Arrhenius($A=(6.25e+26, s^{-1}), n=-3.05, Ea=(96873.7, cal/mol'), T0=(1, K'))$

Current Kinetics

 $\label{eq:arrheniusBM} $$A=(9.04e+06,'m^3/(mol^*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->0_Ext-10-R_N-3R!H->0_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->0_Ext-10-R_N-3R!H->0_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")$

New Current

-10
-30
-40
-50
1.0 1.5 2.0 2.5 3.0

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

Arrhenius($A=(1.34e+27, s^-1')$, n=-3.12, Ea=(91201.3, cal/mol'), T0=(1, K'))

Current Kinetics

ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'k]/mol'), E0=(72.7054,'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-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_1BrCFOS->O_Ext-10-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")

