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

## **New Kinetics:**

Arrhenius( $A=(1.61e+12, s^-1'), n=0.69, Ea=(59688.5, cal/mol'), T0=(1, K')$ 

## **Current Kinetics**

ArrheniusEP(A=(5.92717e+11,'s^-1'), n=0.412677, alpha=0, E0=(186.536,'kJ/mol'), comment="""Average of [Average of [From training reaction 133 used for R3\_D;doublebond\_intra\_pri\_2H;radadd\_intra\_cddouble] + Average of [Average of [Average of [From training reaction 142 used for

R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H]] + Average of [Average of [From training reaction 142 used for R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H] + Average of [From training reaction 142 used for R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H]]] + Average of [Average of [Average of [From training reaction 142 used for

R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H] +
Average of [From training reaction 142 used for
R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H]] +
Average of [Average of [From training reaction 142 used
for R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H]]]
+ Average of [From training reaction 133 used for
R3\_D;doublebond\_intra\_pri\_2H;radadd\_intra\_cddouble]] +
Average of [Average of [Average of [From
training reaction 60 used for

R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]]]
+ Average of [Average of [From training reaction 60 used for

R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]] + Average of [Average of [From training reaction 60 used for R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb] + Average of [From training reaction 60 used for

R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]]]] + Average of [Average of [Average of [From training reaction 142 used for

R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H] + Average of [From training reaction 142 used for R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H]] + Average of [Average of [From training reaction 142 used for R3\_D;doublebond\_intra\_pri\_HCd;radadd\_intra\_cs2H]]] + Average of [Average of [Average of [From training reaction 60 used for

R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]] + Average of [Average of [From training reaction 60 used for R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb] + Average of [From training reaction 60 used for International Control of the Internation 10 used for International Control of Inter

R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]]]

+ From training reaction 135 used for

R3\_D;doublebond\_intra;radadd\_intra\_cs2H + Average of [Average of [Average of [From training reaction 60 used for R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb] + Average of [From training reaction 60 used for

R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]] + Average of [Average of [From training reaction 60 used for R3\_D;doublebond\_intra\_secNd\_2H;radadd\_intra\_csHCb]]]] + Average of [Average of [From training reaction 133 used for

R3\_D;doublebond\_intra\_pri\_2H;radadd\_intra\_cddouble]]] Estimated using template

[R3\_D;doublebond\_intra;radadd\_intra] for rate rule [R3\_D;doublebond\_intra;radadd\_intra\_O] Euclidian distance = 1.0 family: Intra R Add Endocyclic""")

