

Number	Reaction	A	n	E	Ref.
148	$C_4H_6 \rightarrow C_2H_2 + C_2H_3 + H$	1.580E+16	0.00	460	[1]
149	$C_4H_6 \rightarrow 2 C_2H_3$	1.800E+13	0.00	356	[1]
150	$2 C_2H_3 \rightarrow C_4H_6$	1.260E+13	0.00	0	[1]
151	$C_4H_6 + H \rightarrow C_2H_3 + C_2H_4$	5.000E+11	0.00	0	[1]
152	$C_4H_6 + H \rightarrow H_2 + C_2H_2 + C_2H_3$	6.300E+10	0.70	25.1	[1]
153	$C_4H_6 + OH \rightarrow CHO + H + C_3H_5$	5.000E+12	0.00	0	[1]
154	$C_4H_6 + CH_3 \rightarrow CH_4 + C_2H_2 + C_2H_3$	7.000E+13	0.00	77	[1]
155	$C_3H_3 + CH_3 \rightarrow C_4H_6$	5.000E+12	0.00	0	[1]
156	$C_5H_8 \rightarrow C_3H_6 + C_2H_2$	1.000E+16	0.00	305	[1]
157	$C_5H_8 \rightarrow C_3H_4 + C_2H_4$	3.160E+12	0.00	239	[1]
158	$C_5H_8 \rightarrow C_3H_5 + C_2H_3$	3.160E+12	0.00	239	[1]
159	$C_5H_8 + O_2 \rightarrow C_2H_2 + C_3H_5 + HO_2$	3.000E+12	0.00	0	[1]
160	$C_5H_8 + O_2 \rightarrow C_2H_3 + C_3H_4 + HO_2$	3.000E+12	0.00	0	[1]
161	$C_5H_8 + HO_2 \rightarrow C_2H_2 + C_3H_5 + H_2O_2$	1.000E+14	0.00	0	[1]
162	$C_5H_8 + HO_2 \rightarrow C_2H_3 + C_3H_4 + H_2O_2$	1.000E+14	0.00	0	[1]
HP1	$C_7H_{16} \rightarrow CH_3 + 2 C_2H_4 + C_2H_5$	1.000E+18	0.00	357	[2]
HP2	$C_7H_{16} + H \rightarrow H_2 + C_3H_6 + C_2H_4 + C_2H_5$	2.600E+06	2.40	18.7	[2]
HP3	$C_7H_{16} + H \rightarrow H_2 + C_4H_8 + C_2H_4 + CH_3$	2.080E+06	2.40	18.7	[2]
HP4	$C_7H_{16} + H \rightarrow H_2 + 3 C_2H_4 + CH_3$	1.320E+06	2.54	28.3	[2]
HP5	$C_7H_{16} + H \rightarrow H_2 + C_5H_{10} + C_2H_5$	1.300E+06	2.40	18.7	[2]
HP6	$C_7H_{16} + OH \rightarrow H_2O + C_5H_{10} + C_2H_5$	5.460E+06	2.00	-5.5	[2]
HP7	$C_7H_{16} + OH \rightarrow H_2O + C_4H_8 + C_2H_4 + CH_3$	4.380E+06	2.00	-5.5	[2]
HP8	$C_7H_{16} + OH \rightarrow H_2O + C_3H_6 + C_2H_4 + C_2H_5$	4.750E+06	2.00	-2.5	[2]
HP9	$C_7H_{16} + OH \rightarrow H_2O + 3 C_2H_4 + CH_3$	2.180E+07	1.80	4.1	[2]
HP10f	$C_5H_{10} \rightleftharpoons C_3H_5 + C_2H_5$	1.000E+16	0.00	305	[2]
HP11f	$C_5H_{10} \rightleftharpoons C_3H_6 + C_2H_4$	3.160E+12	0.00	239	[2]
HP12	$C_5H_{10} + OH \rightarrow H_2O + C_3H_6 + C_2H_3$	7.080E+07	1.90	0.7	[2]
HP13	$C_5H_{10} + H \rightarrow H_2 + C_3H_6 + C_2H_3$	1.300E+06	2.40	18.7	[2]
HP14	$C_5H_{10} + H \rightarrow 2 C_2H_4 + CH_3$	7.230E+12	0.00	5.4	[2]
HP15f	$C_5H_{10} + H \rightleftharpoons C_3H_6 + C_2H_5$	7.230E+12	0.00	5.4	[2]
HP16	$C_5H_{10} + H \rightarrow H_2 + C_2H_4 + C_3H_5$	6.600E+05	2.54	28.3	[2]
HP17	$C_5H_{10} + H \rightarrow H_2 + C_4H_6 + CH_3$	1.150E+05	2.50	10.4	[2]
HP18	$C_4H_8 \rightarrow C_3H_5 + CH_3$	1.000E+16	0.00	305	[2]
HP19f	$C_4H_8 + H \rightleftharpoons C_2H_4 + C_2H_5$	7.230E+12	0.00	5.4	[2]
HP20f	$C_4H_8 + H \rightleftharpoons C_3H_6 + CH_3$	7.230E+12	0.00	5.4	[2]
HP21	$C_4H_8 + H \rightarrow H_2 + C_2H_3 + C_2H_4$	6.600E+05	2.54	28.3	[2]

Number	Reaction	A	n	E	Ref.
HP22	$\text{C}_4\text{H}_8 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{C}_4\text{H}_6 + \text{H}$	2.080E+06	2.00	-1.2	[2]

Units are mol, cm³, kJ, K.

The backward rates for all reversible reactions can be calculated from thermodynamic data.

References

- [1] S. C. Li, B. Varatharajan, and F. A. Williams. The chemistry of jp-10 ignition. *AIAA Journal*, 39(12):2351–2356, 2001.
- [2] T. J. Held, A. J. Marchese, and F. L. Dryer. A semi-empirical reaction mechanism for n-heptane oxidation and pyrolysis. *Combustion Science and Technology*, 123:107–146, 1997.