

Kinetic mechanism for *n*-heptane autoignition

Number	Reaction	<i>A</i>	<i>n</i>	<i>E</i>
1f	$\text{O}_2 + \text{H} \longrightarrow \text{OH} + \text{O}$	2.000E+14	0.00	70.3
2f	$\text{H}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{H}$	1.000E+08	1.60	13.8
3f	$2\text{OH} \longrightarrow \text{H}_2\text{O} + \text{O}$	1.500E+09	1.14	0.42
4f	$\text{H} + \text{OH} + \text{M}' \longrightarrow \text{H}_2\text{O} + \text{M}'$	2.200E+22	-2.00	0.00
5	$\text{H} + \text{O}_2 + \text{M}' \longrightarrow \text{HO}_2 + \text{M}'$	2.300E+18	-0.80	0.00
6	$\text{HO}_2 + \text{H} \longrightarrow 2\text{OH}$	1.500E+14	0.00	4.2
7	$\text{HO}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{O}_2$	6.000E+13	0.00	0
8	$2\text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{O}_2$	2.500E+11	0.00	-5.2
9f	$\text{H}_2\text{O}_2 + \text{M}' \longrightarrow 2\text{OH} + \text{M}'$	4.424E+24	-2.00	211
10f	$\text{CO} + \text{OH} \longrightarrow \text{CO}_2 + \text{H}$	6.000E+06	1.50	-3.1
11	$\text{CH} + \text{CO}_2 \longrightarrow \text{CHO} + \text{CO}$	3.400E+12	0.00	2.9
12	$\text{CH} + \text{H}_2\text{O} \longrightarrow \text{CH}_2\text{OH}$	5.700E+12	0.00	-3.2
13	$\text{CHO} + \text{M}' \longrightarrow \text{CO} + \text{H} + \text{M}'$	7.100E+14	0.00	70.3
14	$\text{CHO} + \text{H} \longrightarrow \text{CO} + \text{H}_2$	9.000E+13	0.00	0
15	$\text{CHO} + \text{OH} \longrightarrow \text{CO} + \text{H}_2\text{O}$	1.000E+14	0.00	0
16	$3\text{-CH}_2 + \text{H} \longrightarrow \text{CH} + \text{H}_2$	6.000E+12	0.00	-7.5
17	$3\text{-CH}_2 + \text{O}_2 \longrightarrow \text{CO} + \text{OH} + \text{H}$	1.300E+13	0.00	6.2
18	$3\text{-CH}_2 + \text{H}_2 \longrightarrow \text{CH}_3 + \text{H}$	7.200E+13	0.00	0
19	$\text{CH}_2\text{O} + \text{OH} \longrightarrow \text{CHO} + \text{H}_2\text{O}$	3.400E+09	1.20	-1.9
20	$\text{CH}_3 + \text{O} \longrightarrow \text{CH}_2\text{O} + \text{H}$	8.430E+13	0.00	0
21	$\text{CH}_3 + \text{O}_2 \longrightarrow \text{CH}_2\text{O} + \text{OH}$	3.300E+11	0.00	37.4
22	$\text{CH}_3 + \text{H} \longrightarrow \text{CH}_3\text{O} + \text{OH}$	1.800E+13	0.00	0
23	$\text{CH}_3 + \text{H} \longrightarrow \text{CH}_4$	$k_0 = 6.257\text{E}+23$	-1.80	0
		$k_\infty = 2.108\text{E}+14$	0.00	0
24f	$2\text{CH}_3 \longrightarrow \text{C}_2\text{H}_6$	$k_0 = 1.272\text{E}+41$	-7.00	11.6
		$k_\infty = 1.813\text{E}+13$	0.00	0
25	$\text{CH}_3\text{O} + \text{M}' \longrightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105
26	$\text{CH}_2\text{OH} + \text{M}' \longrightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105
27	$\text{CH}_4 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{CH}_3$	1.600E+07	1.83	11.6

28	$C_2H_2 + O \longrightarrow 3\text{-}CH_2 + CO$		1.720E+04	2.80	2.1
29	$C_2H_3 \longrightarrow C_2H_2 + H$	$k_0 =$	1.187E+42	-7.50	190
		$k_\infty =$	2.000E+14	0.00	166
30	$C_2H_3 + O_2 \longrightarrow C_2H_2 + HO_2$		1.210E+11	0.00	0
31	$C_2H_3 + O_2 \longrightarrow CH_2O + CHO$		5.420E+12	0.00	0
32	$C_2H_4 + OH \longrightarrow C_2H_3 + H_2O$		6.500E+13	0.00	24.9
33	$C_2H_4 + H \longrightarrow C_2H_3 + H_2$		1.700E+15	0.00	62.9
34	$C_2H_5 \longrightarrow C_2H_4 + H$	$k_0 =$	1.000E+16	0.00	126
		$k_\infty =$	1.300E+13	0.00	167
35	$C_2H_5 + O_2 \longrightarrow C_2H_4 + HO_2$		1.100E+10	0.00	-6.3
36	$C_2H_6 + H \longrightarrow C_2H_5 + H_2$		1.400E+09	1.50	31.1
37	$C_3H_6 + OH \longrightarrow C_2H_5 + H_2$		7.900E+12	0.00	0
38	$n\text{-}C_3H_7 \longrightarrow CH_3 + C_2H_4$		9.600E+13	0.00	130
39f	$n\text{-}C_3H_7 \longrightarrow H + C_3H_6$		1.250E+14	0.00	155
40	$n\text{-}C_3H_7 + O_2 \longrightarrow C_3H_6 + HO_2$		1.000E+12	0.00	20.9
41	$p\text{-}C_4H_9 \longrightarrow C_2H_5 + C_2H_4$		2.500E+13	0.00	121
42	$1\text{-}C_5H_{11} \longrightarrow C_2H_4 + n\text{-}C_3H_7$		3.200E+13	0.00	119
43	$1\text{-}C_7H_{15} \longrightarrow 1\text{-}C_5H_{11} + C_2H_4$		1.500E+13	0.00	121
44	$2\text{-}C_7H_{15} \longrightarrow p\text{-}C_4H_9 + C_3H_6$		5.600E+13	0.00	118
45	$n\text{-}C_7H_{16} \longrightarrow p\text{-}C_4H_9 + n\text{-}C_3H_7$		3.160E+16	0.00	339
46	$n\text{-}C_7H_{16} + H \longrightarrow 1\text{-}C_7H_{15} + H_2$		5.600E+07	2.00	32.2
47	$n\text{-}C_7H_{16} + H \longrightarrow 2\text{-}C_7H_{15} + H_2$		4.378E+07	2.00	20.9
48	$n\text{-}C_7H_{16} + OH \longrightarrow 1\text{-}C_7H_{15} + H_2O$		8.610E+09	1.10	7.6
49	$n\text{-}C_7H_{16} + OH \longrightarrow 2\text{-}C_7H_{15} + H_2O$		6.500E+07	1.30	2.9
50	$n\text{-}C_7H_{16} + HO_2 \longrightarrow 1\text{-}C_7H_{15} + H_2O_2$		1.120E+13	0.00	81.2
51	$n\text{-}C_7H_{16} + HO_2 \longrightarrow 2\text{-}C_7H_{15} + H_2O_2$		1.675E+13	0.00	71.2
52	$n\text{-}C_7H_{16} + O_2 \longrightarrow 1\text{-}C_7H_{15} + HO_2$		2.500E+13	0.00	205
53	$n\text{-}C_7H_{16} + O_2 \longrightarrow 2\text{-}C_7H_{15} + HO_2$		1.000E+14	0.00	199
54f	$1\text{-}C_7H_{15} + O_2 \longrightarrow 1\text{-}C_7H_{15}O_2$		2.000E+12	0.00	0
55f	$2\text{-}C_7H_{15} + O_2 \longrightarrow 1\text{-}C_7H_{15}O_2$		2.000E+12	0.00	0
56f	$1\text{-}C_7H_{15}O_2 \longrightarrow C_7H_{15}O_2$		2.000E+11	0.00	71.2
57	$C_7H_{15}O_2 + O_2 \longrightarrow OOC_7H_{14}OOH$		5.000E+11	0.00	0

58	$\text{OOC}_7\text{H}_{14}\text{OOH} \longrightarrow \text{HOOC}_7\text{H}_{13}\text{OOH}$	2.000E+11	0.00	71.2
59	$\text{HOOC}_7\text{H}_{13}\text{OOH} \longrightarrow \text{OC}_7\text{H}_{13}\text{OOH} + \text{OH}$	1.000E+09	0.00	31.4
60	$\text{OC}_7\text{H}_{13}\text{OOH} \longrightarrow \text{OC}_7\text{H}_{13}\text{O} + \text{OH}$	8.400E+14	0.00	180
61	$\text{OC}_7\text{H}_{13}\text{O} \longrightarrow \text{CH}_2\text{O} + 1\text{-C}_5\text{H}_{11} + \text{CO}$	2.000E+13	0.00	62.8

Units are mole, cubic centimeter, second, kilojoule, kelvin.

Rate constants are written as $AT^n \exp(-E/RT)$.

Third body collision efficiencies are $[\text{M}'] = 3.0[n\text{-C}_7\text{H}_{16}] + 1.0[\text{H}_2] + 0.75[\text{CO}] + 0.40[\text{N}_2] + 6.5[\text{H}_2\text{O}] + 0.4[\text{O}_2]$.

For those rate constants k , which depend on the pressure, k_0 and k_∞ are given in the table and $k = Fk_0[\text{M}]/(k_\infty + k_0[\text{M}])$, where $\log_{10}F = \log_{10}F_C / (1 + (\log_{10}(k_0[\text{M}] / k_\infty) / \hat{N})^2)$ and $\hat{N} = 0.75 - 1.27 \log_{10}F_C$.

Broadening functions are given by $F_{C23} = 0.577 \exp(-T / 2370 \text{ K})$, $F_{C24} = 0.38 \exp(-T / 73 \text{ K}) + 0.62 \exp(-T / 1180 \text{ K})$, $F_{C29} = 0.35$ and $F_{C34} = 0.411 \exp(-T / 73.4 \text{ K}) + \exp(-T / 422.8 \text{ K})$.

Thermochemical data

	A_1	A_2	A_3	A_4	A_5	A_6	A_7
N ₂	2.93E+00	1.49E-03	-5.68E-07	1.01E-10	-6.75E-15	-9.23E+02	5.98E+00
O ₂	3.70E+00	6.14E-04	-1.26E-07	1.78E-11	-1.14E-15	-1.23E+03	3.19E+00
H	2.50E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.55E+04	-4.60E-01
OH	2.88E+00	1.01E-03	-2.28E-07	2.17E-11	-5.13E-16	3.89E+03	5.60E+00
O	2.54E+00	-2.76E-05	-3.10E-09	4.55E-12	-4.37E-16	2.92E+04	4.92E+00
H ₂	2.99E+00	7.00E-04	-5.63E-08	-9.23E-12	1.58E-15	-8.35E+02	-1.36E+00
H ₂ O	2.67E+00	3.06E-03	-8.73E-07	1.20E-10	-6.39E-15	-2.99E+04	6.86E+00
HO ₂	4.17E+00	1.88E-03	-3.46E-07	1.95E-11	1.76E-16	6.18E+01	2.96E+00
H ₂ O ₂	4.57E+00	4.34E-03	-1.47E-06	2.35E-10	-1.43E-14	-1.80E+04	5.01E-01
CO	3.03E+00	1.44E-03	-5.63E-07	1.02E-10	-6.91E-15	-1.43E+04	6.11E+00
CO ₂	4.45E+00	3.14E-03	-1.28E-06	2.39E-10	-1.67E-14	-4.90E+04	-9.55E-01
CH	2.52E+00	1.77E-03	-4.61E-07	5.93E-11	-3.35E-15	7.11E+04	7.41E+00
CHO	3.56E+00	3.35E-03	-1.34E-06	2.47E-10	-1.71E-14	3.92E+03	5.55E+00
CH ₂ OH	4.68E+00	6.56E-03	-2.26E-06	3.55E-10	-2.08E-14	-2.89E+03	4.80E-01
3-CH ₂	3.64E+00	1.93E-03	-1.69E-07	-1.01E-10	1.81E-14	4.53E+04	2.16E+00
CH ₃	2.84E+00	6.14E-03	-2.23E-06	3.79E-10	-2.45E-14	1.64E+04	5.45E+00
CH ₂ O	3.17E+00	6.19E-03	-2.25E-06	3.66E-10	-2.20E-14	-1.45E+04	6.04E+00
CH ₃ O	3.77E+00	7.87E-03	-2.66E-06	3.94E-10	-2.11E-14	1.28E+02	2.93E+00
CH ₄	1.68E+00	1.02E-02	-3.88E-06	6.79E-10	-4.50E-14	-1.01E+04	9.62E+00
C ₂ H ₆	4.83E+00	1.38E-02	-4.56E-06	6.72E-10	-3.60E-14	-1.27E+04	-5.24E+00
C ₂ H ₂	4.44E+00	5.38E-03	-1.91E-06	3.29E-10	-2.16E-14	2.57E+04	-2.80E+00
C ₂ H ₃	5.93E+00	4.02E-03	-3.97E-07	-1.44E-10	2.38E-14	3.39E+04	-8.53E+00
C ₂ H ₄	3.53E+00	1.15E-02	-4.42E-06	7.84E-10	-5.27E-14	4.43E+03	2.23E+00
C ₂ H ₅	4.29E+00	1.24E-02	-4.41E-06	7.07E-10	-4.20E-14	1.21E+04	8.46E-01
C ₃ H ₆	6.72E+00	1.49E-02	-4.97E-06	7.25E-10	-3.80E-14	-9.25E+02	-1.22E+01
<i>n</i> -C ₃ H ₇	7.70E+00	1.60E-02	-5.28E-06	7.63E-10	-3.94E-14	8.30E+03	-1.55E+01
<i>p</i> -C ₄ H ₉	6.46E+00	2.58E-02	-8.20E-06	1.24E-09	-7.28E-14	5.19E+03	-5.71E+00
1-C ₅ H ₁₁	1.07E+01	3.09E-02	-1.18E-05	2.06E-09	-1.34E-13	1.92E+01	-2.75E+01
2-C ₇ H ₁₅	1.49E+01	4.32E-02	-1.66E-05	2.93E-09	-1.93E-13	-7.18E+03	-4.68E+01
1-C ₇ H ₁₅	1.49E+01	4.32E-02	-1.66E-05	2.93E-09	-1.93E-13	-7.18E+03	-4.68E+01
<i>n</i> -C ₇ H ₁₆	2.28E+01	3.25E-02	-1.11E-05	1.71E-09	-9.62E-14	-3.37E+04	-9.43E+01
C ₇ H ₁₅ O ₂	2.85E+00	1.60E-03	-6.29E-07	1.14E-10	-7.81E-15	-8.90E+02	6.40E+00
HC ₇ H ₁₄ O ₂	2.85E+00	1.60E-03	-6.29E-07	1.14E-10	-7.81E-15	-8.90E+02	6.40E+00
C ₇ H ₁₅ O ₄	2.85E+00	1.60E-03	-6.29E-07	1.14E-10	-7.81E-15	-8.90E+02	6.40E+00
HC ₇ H ₁₄ O ₄	2.85E+00	1.60E-03	-6.29E-07	1.14E-10	-7.81E-15	-8.90E+02	6.40E+00
C ₇ H ₁₄ O ₃	2.85E+00	1.60E-03	-6.29E-07	1.14E-10	-7.81E-15	-8.90E+02	6.40E+00
OC ₇ H ₁₃ O	2.85E+00	1.60E-03	-6.29E-07	1.14E-10	-7.81E-15	-8.90E+02	6.40E+00

	a_1	a_2	a_3	a_4	a_5	a_6	a_7
N ₂	3.30E+00	1.41E-03	-3.96E-06	5.64E-09	-2.44E-12	-1.02E+03	3.95E+00
O ₂	3.21E+00	1.13E-03	-5.76E-07	1.31E-09	-8.77E-13	-1.01E+03	6.03E+00
H	2.50E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.55E+04	-4.60E-01
OH	3.64E+00	1.85E-04	-1.68E-06	2.39E-09	-8.43E-13	3.61E+03	1.36E+00
O	2.95E+00	-1.64E-03	2.42E-06	-1.60E-09	3.89E-13	2.91E+04	2.96E+00
H ₂	3.30E+00	8.25E-04	-8.14E-07	-9.48E-11	4.13E-13	-1.01E+03	-3.29E+00
H ₂ O	3.39E+00	3.47E-03	-6.35E-06	6.97E-09	-2.51E-12	-3.02E+04	2.59E+00
HO ₂	4.30E+00	-4.75E-03	2.12E-05	-2.43E-08	9.29E-12	2.95E+02	3.72E+00
H ₂ O ₂	3.39E+00	6.57E-03	-1.49E-07	-4.63E-09	2.47E-12	-1.77E+04	6.79E+00
CO	3.26E+00	1.51E-03	-3.88E-06	5.58E-09	-2.47E-12	-1.43E+04	4.85E+00
CO ₂	2.28E+00	9.92E-03	-1.04E-05	6.87E-09	-2.12E-12	-4.84E+04	1.02E+01
CH	3.49E+00	3.24E-04	-1.69E-06	3.16E-09	-1.41E-12	7.08E+04	2.08E+00
CHO	2.90E+00	6.20E-03	-9.62E-06	1.09E-08	-4.57E-12	4.16E+03	8.98E+00
CH ₂ OH	3.86E+00	5.59E-03	5.95E-06	-1.05E-08	4.38E-12	-2.51E+03	5.47E+00
3-CH ₂	3.76E+00	1.16E-03	2.49E-07	8.80E-10	-7.33E-13	4.54E+04	1.71E+00
CH ₃	2.43E+00	1.11E-02	-1.68E-05	1.62E-08	-5.86E-12	1.64E+04	6.79E+00
CH ₂ O	4.79E+00	-9.91E-03	3.73E-05	-3.79E-08	1.32E-11	-1.43E+04	6.03E-01
CH ₃ O	2.11E+00	7.22E-03	5.34E-06	-7.38E-09	2.08E-12	9.79E+02	1.32E+01
CH ₄	7.79E-01	1.75E-02	-2.78E-05	3.05E-08	-1.22E-11	-9.83E+03	1.37E+01
C ₂ H ₆	1.46E+00	1.55E-02	5.78E-06	-1.26E-08	4.59E-12	-1.12E+04	1.44E+01
C ₂ H ₂	2.01E+00	1.52E-02	-1.62E-05	9.08E-09	-1.91E-12	2.61E+04	8.81E+00
C ₂ H ₃	2.46E+00	7.37E-03	2.11E-06	-1.32E-09	-1.18E-12	3.54E+04	1.16E+01
C ₂ H ₄	-8.61E-01	2.80E-02	-3.39E-05	2.79E-08	-9.74E-12	5.57E+03	2.42E+01
C ₂ H ₅	4.31E+00	-4.18E-03	4.97E-05	-5.99E-08	2.30E-11	1.28E+04	4.71E+00
C ₃ H ₆	1.46E+00	2.11E-02	4.05E-06	-1.63E-08	7.05E-12	1.07E+03	1.74E+01
<i>n</i> -C ₃ H ₇	1.05E+00	2.60E-02	2.38E-06	-1.96E-08	9.37E-12	1.06E+04	2.11E+01
<i>p</i> -C ₄ H ₉	2.59E-01	4.62E-02	-3.05E-05	9.74E-09	-5.38E-13	6.56E+03	2.51E+01
1-C ₅ H ₁₁	2.20E+00	4.13E-02	6.59E-06	-3.38E-08	1.54E-11	3.02E+03	1.94E+01
2-C ₇ H ₁₅	2.47E+00	5.89E-02	9.51E-06	-4.87E-08	2.21E-11	-2.82E+03	2.21E+01
1-C ₇ H ₁₅	2.47E+00	5.89E-02	9.51E-06	-4.87E-08	2.21E-11	-2.82E+03	2.21E+01
<i>n</i> -C ₇ H ₁₆	3.01E+00	5.45E-02	2.18E-05	-5.42E-08	2.08E-11	-2.60E+04	1.75E+01
C ₇ H ₁₅ O ₂	3.70E+00	-1.42E-03	2.87E-06	-1.20E-09	-1.40E-14	-1.06E+03	2.23E+00
HC ₇ H ₁₄ O ₂	3.70E+00	-1.42E-03	2.87E-06	-1.20E-09	-1.40E-14	-1.06E+03	2.23E+00
C ₇ H ₁₅ O ₄	3.70E+00	-1.42E-03	2.87E-06	-1.20E-09	-1.40E-14	-1.06E+03	2.23E+00
HC ₇ H ₁₄ O ₄	3.70E+00	-1.42E-03	2.87E-06	-1.20E-09	-1.40E-14	-1.06E+03	2.23E+00
C ₇ H ₁₄ O ₃	3.70E+00	-1.42E-03	2.87E-06	-1.20E-09	-1.40E-14	-1.06E+03	2.23E+00
OC ₇ H ₁₃ O	3.70E+00	-1.42E-03	2.87E-06	-1.20E-09	-1.40E-14	-1.06E+03	2.23E+00

Species formula:

$$c_{p0}/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$H_0/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$S_0/R = a_1 \ln T + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

a_1 - a_2 are the coefficients A_1 - A_7 and a_1 - a_7 depending on the temperature range:

a_1 - a_7 : for the low temperature interval ($T < 1000$ K)

A_1 - A_7 : for the high temperature interval ($T \geq 1000$ K)