$CH_3CH_2CH_2CH_2O + O_2 \rightarrow CH_3CH_2CH_2CHO + HO_2$

$\Delta H° = -127.4$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
7.7 x 10^{-15}	298	Hoffmann et al., 1992	PLP-LIF (a)
(1.4 ± 0.7) x 10^{-14}	293	Hein et al., 1999	PLP-AS/LIF (b)
Relative Rate Coefficients			
6.8 x 10^{-13} exp[-(1178 ± 176)/T]	265-393	Morabito and Heicklen, 1987	RR (c)
1.3 x 10^{-14}	298		

Comments

(a) Pulsed laser photolysis of Cl$_2$ in the presence of *n*-C$_4$H$_{10}$-O$_2$-NO mixtures in a flow system at total pressures of 10 mbar to 50 mbar of N$_2$ (13 Torr to 67 Torr). Time-resolved monitoring of OH radicals was carried out by cw-laser absorption, and of NO$_2$ by LIF. The rate coefficient was derived from a computer simulation of OH radical and NO$_2$ temporal profiles.

(b) Pulsed laser photolysis at 248 nm of a mixture of 1-bromobutane, O$_2$ and NO in N$_2$ at 50 mbar total pressure in a slow-flow system. OH and NO$_2$ were monitored in real-time using laser long-path absorption at 308.417 nm and cw laser-excited fluorescence after excitation at 488 nm, respectively. The rate coefficient was derived from a computer simulation of the OH and NO$_2$ temporal concentration profiles.

(c) Photolysis of 1-butyl nitrite at 366 nm in the presence of NO and O$_2$. Rate data were derived from the quantum yields of product formation, and a rate coefficient ratio of k(1-C$_4$H$_9$O + O$_2$)/k(1-C$_4$H$_9$O + NO) = 1.67 x 10^{-2} exp[-(1178 ± 176)/T] was obtained. This rate coefficient ratio is placed on an absolute basis using a rate cofficient of k(1-C$_4$H$_9$O + NO) = 4.1 x 10^{-11} cm^3 molecule^{-1} s^{-1}, independent of temperature (see data sheet for 2-C$_3$H$_7$O + NO, this evaluation).

Preferred Values

k = 1.4 x 10^{-14} cm^3 molecule^{-1} s^{-1} at 298 K.
k = 8.9 x 10^{-14} exp(-550/T) cm^3 molecule^{-1} s^{-1} over the range 250 to 350 K.

Reliability
   Δlog k = ± 0.3 at 298 K.
   $\Delta(E/R)$ = ± 300 K.

Comments on Preferred Values

k(298 K) based on the indirect study of Hein *et al.* which is in good agreement with the relative rate technique by Morabito and Heicklen at 298 K. Temperature dependence adopts (*E/R*) estimated by Atkinson (1997), based on available data for smaller alkoxy radicals, and an A-factor to give the preferred value at 298 K.

References

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