Website: http://iupac.pole-ether.fr. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.
This data sheet updated: 12th November 2002.

$$HOCH_2CH_2O_2 + HOCH_2CH_2O_2 \rightarrow HOCH_2CH_2OH + HOCH_2CHO + O_2 \quad (1)$$
$$\rightarrow 2\ HOCH_2CH_2O + O_2 \quad\quad\quad\quad\quad (2)$$

Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.2 \pm 0.3) \times 10^{-12}$	296	Murrells *et al.*, 1991[1]	PLP/MM-UVAS (a,b)
$(2.1 \pm 0.3) \times 10^{-12}$	298	Jenkin and Hayman, 1995[2]	MM-UVAS (a,c)
$7.8 \times 10^{-14} \exp[(1000 \pm 80)/T]$	300-470	Boyd and Lesclaux, 1997[3]	PLP-UVAS (a,d)
$(2.2 \pm 0.3) \times 10^{-12}$	298		
Branching Ratios			
$k_2/k = (0.5 \pm 0.1)$	298	Barnes, Becker, and Ruppert, 1993[4]	P-FTIR (e)
$k_2/k = 0.55$	298	Boyd and Lesclaux, 1997[3]	PLP-UVAS (f)

Comments

(a) k is defined by $-d[HOCH_2CH_2O_2]/dt = 2k[HOCH_2CH_2O_2]^2$.

(b) Separate pulsed laser photolysis and molecular modulation studies using the photolysis of H_2O_2 to produce OH radicals in the presence of ethene and air at a pressure of 1 bar (760 Torr). $HOCH_2CH_2O_2$ radicals were monitored by UV absorption at 250 nm with $\sigma_{250} = 4.7 \times 10^{-18}$ cm^2 molecule^{-1} (mean value). $k_{obs}/\sigma_{250} = 6.7 \times 10^5$ cm s^{-1}. k was calculated from the laser photolysis experiments with $k_2/k = 0.36$.

(c) Identical technique to that in note (a). $k_{obs}/\sigma_{250} = (7.1 \pm 0.6) \times 10^5$ cm s^{-1}. k calculated using $k_2/k = 0.5$ and, in addition, using data from ref. 1.

(d) Pulsed laser photolysis of H_2O_2 at 248 nm in the presence of ethene and O_2. $HOCH_2CH_2O_2$ radicals were monitored by absorption at 250 nm.

(e) Analysis of products by FTIR in the photolysis of $HOCH_2CH_2I$ or H_2O_2-C_2H_4 mixtures in O_2 + N_2. Pressure 150 mbar to 900 mbar (114 Torr to 680 Torr). Mean value given from both systems, which were in excellent agreement, and independent of total pressure or O_2 concentration.

(f) Based on HO$_2$ radical formation from the $HOCH_2CH_2O + O_2$ reaction, measured by UV absorption at 220 nm.

Preferred Values

$k = 2.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 7.8 \times 10^{-14} \exp(1000/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 250 K to 450 K.
$k_2/k = 0.5$ at 298 K.

Reliability
  $\Delta \log k = \pm 0.1$ at 298 K.

$\Delta(E/R) = \pm300$ K.

$\Delta(k_2/k) = \pm0.1$ at 298 K.

Comments on Preferred Values

All the recent studies of this reaction provide consistent and seemingly reliable values for the rate coefficient and for the branching ratio.[1,3] The preferred value of k at 298 K is a mean of the values reported by Murrells *et al.*,[1] Jenkin and Hayman[2] and Boyd and Lesclaux,[3] and for the branching ratio the value of Barnes *et al.*[4] is accepted. The temperature dependence of k from the work of Boyd and Lesclaux,[3] is recommended but with wider error limits on E/R. A measurement of the temperature dependence of the branching ratio would be of value.

References

[1] T. P. Murrells, M. E. Jenkin, S. J. Shalliker, and G. D. Hayman, J. Chem. Soc. Faraday Trans. **87**, 2351 (1991).

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[4] I. Barnes, K. H. Becker, and L. Ruppert, Chem. Phys. Lett. **203**, 295 (1993).