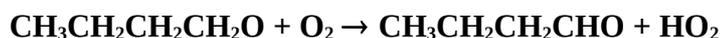


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_5

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: 16th November 2006.



$$\Delta H^\circ = -127.4 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

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

Comments

- Pulsed laser photolysis of Cl_2 in the presence of $n\text{-C}_4\text{H}_{10}\text{-O}_2\text{-NO}$ 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.
- 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.
- 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 $k(1\text{-C}_4\text{H}_9\text{O} + \text{O}_2)/k(1\text{-C}_4\text{H}_9\text{O} + \text{NO}) = 1.67 \times 10^{-2} \exp[-(1178 \pm 176)/T]$ was obtained. This rate coefficient ratio is placed on an absolute basis using a rate coefficient of $k(1\text{-C}_4\text{H}_9\text{O} + \text{NO}) = 4.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature (see data sheet for $2\text{-C}_3\text{H}_7\text{O} + \text{NO}$, this evaluation).

Preferred Values

$$k = 1.4 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 8.9 \times 10^{-14} \exp(-550/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the range } 250 \text{ to } 350 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.3 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 300 \text{ K.}$$

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

- Atkinson, R., J. Phys. Chem. Ref. Data, 26, 215, 1997; Int. J. Chem. Kinet., 29, 99, 1997.
Hoffmann, A., Mörs, V. and Zellner, R.: Ber. Bunsenges. Phys. Chem. 96, 437, 1992.
Hein, H., Hoffmann, A. and Zellner, R.: Phys. Chem. Chem. Phys. 1, 3743, 1998.
Morabito, P. and Heicklen, J.: Bull. Chem. Soc. Jpn 60, 2641, 1987.