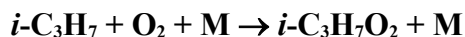


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet R_Oxygen_6

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 June 2003.



$$\Delta H^\circ = -158.9 \text{ kJ}\cdot\text{mol}^{-1}$$

High-pressure rate coefficients

Rate coefficient data

$k_\infty/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.41 \pm 0.24) \times 10^{-11}$	298	Ruiz and Bayes, 1984 ¹	FP-MS (a)
8.3×10^{-12}	300	Munk <i>et al.</i> , 1986 ²	(b)

Comments

- (a) No pressure dependence detected for He or N₂ pressures from 1.3 mbar to 5 mbar.
- (b) Pulsed radiolysis in H₂ at 1 bar. *i*-C₃H₇ radicals were generated by the addition of H atoms to C₃H₆ and *i*-C₃H₇O₂ detected by UV absorption at 253 nm. Absorption spectrum of *i*-C₃H₇ was also detected.

Preferred Values

$k \approx k_\infty$ at 298 K and 1 bar of air.

$k_\infty = 1.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range 200 K to 300 K.

Reliability

$\Delta \log k_\infty = \pm 0.3$ over the range 200 K to 300 K.

Comments on Preferred Values

The preferred values are the average of the results from refs. 1 and 2. Falloff corrections are probably within the uncertainties of the average. The rate coefficient k_∞ for this reaction appears consistent with those for the reactions $\text{C}_2\text{H}_5 + \text{O}_2 + \text{M} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{M}$ and $n\text{-C}_3\text{H}_7 + \text{O}_2 + \text{M} \rightarrow n\text{-C}_3\text{H}_7\text{O}_2 + \text{M}$ (see this evaluation).

References

- ¹ R. P. Ruiz and K. D. Bayes, *J. Phys. Chem.* **88**, 2592 (1984).
- ² J. Munk, P. Pagsberg, E. Ratajczak, and A. Sillesen, *Chem. Phys. Lett.* **132**, 417 (1986).