

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_VOC46

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This data sheet last evaluated: 2nd August 2007; no revision of preferred values.

HO + CH₃CH₂C(O)CH₂ONO₂ → products

Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | Temp./K | Reference | Technique/ Comments |
|--|---------|------------------|---------------------|
| <i>Relative Rate Coefficients</i> (8.21 ± 1.38) × 10 ⁻¹³ | 298 ± 2 | Zhu et al., 1991 | RR (a) |

Comments

- (a) HO radicals were generated by the photolysis of CH₃ONO-NO-N₂-O₂ mixtures at 1 bar pressure. The concentrations of CH₃CH₂C(O)CH₂ONO₂ and *n*-butane were measured during the experiments by GC, and the measured rate constant ratio of $k(\text{HO} + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_2\text{ONO}_2)/k(\text{HO} + n\text{-butane}) = 0.357 \pm 0.060$ is placed on an absolute basis by use of a rate coefficient of $k(\text{HO} + n\text{-butane}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation).

Preferred Values

$$k = 8.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

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

Comments on Preferred Values

The preferred value is based on the sole study of Zhu et al. (1991), but with a higher uncertainty.

References

IUPAC,; <http://iupac.pole-ether.fr>, 2013.

Zhu, T., Barnes, I. and Becker, K. H.: J. Atmos. Chem. 13, 301, 1991.