IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC45

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

HO + $CH_3C(O)CH_2ONO_2$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$<4.0 \times 10^{-13}$	298 ± 2	Zhu et al., 1991	RR (a)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO-NO-N_2-O_2 mixtures at 1 bar pressure. The concentrations of $CH_3C(O)CH_2ONO_2$ and *n*-butane were measured during the experiments by GC, and the measured rate constant ratio of $k(HO + CH_3C(O)CH_2ONO_2)/k(HO + n\text{-butane}) < 0.17$ is placed on an absolute basis by use of a rate coefficient of $k(HO + n\text{-butane}) = 2.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

Preferred Values

$k < 1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

The preferred value is based on the sole study of Zhu et al. (1991), but with a higher upper limit to reflect additional uncertainties.

References

IUPAC,: http://iupac.pole-ether.fr, 2013.
Zhu, T., Barnes, I. and Becker, K. H.: J. Atmos. Chem. 13, 301, 1991.