IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM13

This data sheet last evaluated November 2008; last change in preferred values November 2008.

HO + 6-methyl-2-nitrophenol → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients $(2.76 \pm 0.18) \times 10^{-12}$	296 ± 3	Bejan et al., 2007	RR (a)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO. Experiments were carried out in a 1080 L chamber at 1.013 bar of air. The concentrations of 6-methyl-2-nitrophenol and ethene (the reference compound) were measured by FTIR spectroscopy. Wall losses and photolysis of 6-methyl-2-nitrophenol were measured and taken into account in the data analysis, and these contributed ~50-55% of the total measured 6-methyl-2-nitrophenol loss rate during the experiments. The measured rate coefficient ratio of k(HO + 6-methyl-2-nitrophenol)/k(HO + ethene) = 0.32 ± 0.02 is placed on an absolute basis by use of a rate coefficient at 296 K and atmospheric pressure of air of k(HO + ethene) = 8.61×10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003).

Preferred Values

$k = 2.8 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

Comments on Preferred Values

The 298 K preferred value is based on the sole reported study of Bejan et al. (2007).

References

Atkinson, R. and Arey, J.: Chem. Rev., 103, 4605, 2003.
Bejan, I., Barnes, I., Olariu, R., Zhou, S., Wiesen, P. and Benter, Th.: Phys. Chem. Chem. Phys., 9, 5686, 2007.