

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_AROM10

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

HO + 3-methyl-2-nitrophenol → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> $(3.70 \pm 0.18) \times 10^{-12}$	296 ± 3	Bejan et al., 2007	RR (a)

Comments

- (a) HO radicals were generated by the photolysis of CH₃ONO. Experiments were carried out in a 1080 L chamber at 1.013 bar of air. The concentrations of 3-methyl-2-nitrophenol and ethene (the reference compound) were measured by FTIR spectroscopy. Wall losses and photolysis of 3-methyl-2-nitrophenol were measured and taken into account in the data analysis, and these contributed ~50-55% of the total measured 3-methyl-2-nitrophenol loss rate during the experiments. The measured rate coefficient ratio of $k(\text{HO} + 3\text{-methyl-2-nitrophenol})/k(\text{HO} + \text{ethene}) = 0.43 \pm 0.02$ is placed on an absolute basis by use of a rate coefficient at 296 K and atmospheric pressure of air of $k(\text{HO} + \text{ethene}) = 8.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).

Preferred Values

$$k = 3.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

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

Comments on Preferred Values

The 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.