IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC75

This data sheet last evaluated: June 2016; last change in preferred values: June 2016.

HO + $CH_3CH(OH)CH_2ONO_2$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(5.1 \pm 1.0) \times 10^{-12}$	296 ± 2	Treves and Rudich, 2003	RR (a, b)

Comments

(a) The rate coefficient was measured at atmospheric pressure of dry synthetic air in a photochemical reactor (100 L Tedlar chamber) by the relative rate technique using solid-phase microextraction (SPME) coupled to gas chromatography (GC) for the detection of the organic reactants. HO radicals were generated by the photolysis of CH_3ONO (or C_2H_5ONO)-NO-air + 1-nitrooxy-2-propanol + 1-pentanol (or 1-octanol) mixtures at wavelengths > 300 nm. The measured rate coefficient ratios of k(HO + 1-nitrooxy-2-propanol)/k(HO + 1-pentanol) and k(HO + 1-nitrooxy-2-propanol)/k(HO + 1-octanol) were not given by the authors, they were placed on an absolute basis using k(HO + 1-pentanol) = $(1.12 \pm 0.15) \times 10^{-11}$ and k(HO + 1-octanol) = $(1.44 \pm 0.15) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Nelson et al., 1990).

(b) Average of the data obtained relative to HO + 1-pentanol and HO + 1-octanol.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	5.1×10^{-12}	298
Reliability		
$\Delta \log k$	± 0.2	298

Comments on Preferred Values

The preferred value is an average of the relative rate coefficients of Treves and Rudich (2003) obtained with two reference compounds. The reaction of OH with $CH_3CH(OH)CH_2ONO_2$ is expected to proceed mainly via H-atom abstraction from the CH

group in the α-position to the hydroxyl group leading to $CH_3C(OH)CH_2ONO_2$ radicals which would reacts with O_2 leading to HO_2 and nitro-oxy acetone ($CH_3C(O)CH_2ONO_2$).

$$HO + CH_3CH(OH)CH_2ONO_2 \rightarrow CH_3C(OH)CH_2ONO_2 + H_2O \quad (1)$$
$$O_2 + CH_3C(OH)CH_2ONO_2 \rightarrow CH_3C(O)CH_2ONO_2 + HO_2 \quad (2)$$

References

Nelson, L., Rattigan, O., Neavyn, R., Sidebottom, H., Treacy, J., and Nielsen, O.J.: Int. J. Chem. Kinet., 22, 1111, 1990.
Treves, K., and Rudich, Y.: J. Phys. Chem. A, 107, 7809, 2003.