

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO<sub>x</sub>\_VOC74

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

### HO + CH<sub>3</sub>CH(ONO<sub>2</sub>)CH<sub>2</sub>OH → products

#### Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $T/\text{K}$ | Reference               | Technique/<br>Comments |
|--|--------------|-------------------------|------------------------|
| <i>Relative Rate Coefficients</i>                    |              |                         |                        |
| $(6.7 \pm 1.3) \times 10^{-12}$                      | $296 \pm 2$  | 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<sub>3</sub>ONO (or C<sub>2</sub>H<sub>5</sub>ONO)-NO-air + 2-nitrooxy-1-propanol + 1-pentanol (or 1-octanol) mixtures at wavelengths > 300 nm. The measured rate coefficient ratios of  $k(\text{HO} + 2\text{-nitrooxy-1-propanol})/k(\text{HO} + 1\text{-pentanol})$  and  $k(\text{HO} + 2\text{-nitrooxy-1-propanol})/k(\text{HO} + 1\text{-octanol})$  were not given by the authors, they were placed on an absolute basis using  $k(\text{HO} + 1\text{-pentanol}) = (1.12 \pm 0.15) \times 10^{-11}$  and  $k(\text{HO} + 1\text{-octanol}) = (1.44 \pm 0.15) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Nelson et al., 1990).
- (b) Average of the data obtained relative to HO + 1-pentanol and HO + 1-octanol.

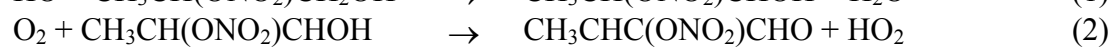
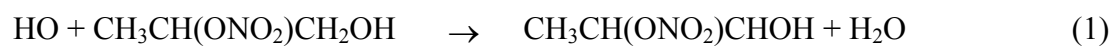
#### Preferred Values

| Parameter  | Value                 | $T/\text{K}$ |
|--|-----------------------|--------------|
| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $6.7 \times 10^{-12}$ | 298          |
| <i>Reliability</i>                                   |                       |              |
| $\Delta \log k$                                      | $\pm 0.2$             | 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<sub>3</sub>CH(ONO<sub>2</sub>)CH<sub>2</sub>OH is expected to proceed mainly via H-atom abstraction from the -CH<sub>2</sub> group in the  $\alpha$ -position to the hydroxyl group leading to CH<sub>3</sub>CH(ONO<sub>2</sub>)CHOH

radicals, which would react with O<sub>2</sub> leading to HO<sub>2</sub> and the corresponding carbonyl (CH<sub>3</sub>CH(ONO<sub>2</sub>)CHO).



### 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.