

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO<sub>x</sub>\_VOC71

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### HO + HOCH<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/ Comments
<i>Relative Rate Coefficients</i>			
$(1.36 \pm 0.13) \times 10^{-11}$	$296 \pm 2$	Aschmann and Atkinson, 1998	RR (a, b)
$(1.54 \pm 0.14) \times 10^{-11}$	$296 \pm 2$	Aschmann and Atkinson, 1998	RR (a, c)

#### Comments

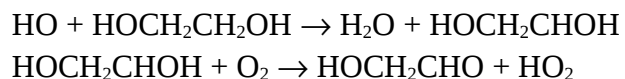
- (a) Relative rate method carried out at atmospheric pressure of air. HO radicals were generated by the photolysis of CH<sub>3</sub>ONO-NO-air + 1,2-ethanediol + *m*-xylene + cyclohexane mixtures at wavelengths > 300 nm. The concentrations of HOCH<sub>2</sub>CH<sub>2</sub>OH, cyclohexane and *m*-xylene (the reference compounds) were measured during the experiments by gas chromatography with flame ionization detection (GC-FID). The measured rate coefficient ratios of  $k(\text{HO} + \text{HOCH}_2\text{CH}_2\text{OH})/k(\text{HO} + \text{cyclohexane}) = 1.96 \pm 0.18$  and  $k(\text{HO} + \text{HOCH}_2\text{CH}_2\text{OH})/k(\text{HO} + \textit{m}\text{-xylene}) = 0.667 \pm 0.062$  are placed on an absolute basis using  $k(\text{HO} + \text{cyclohexane}) = 6.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Calvert et al., 2008) and  $k(\text{HO} + \textit{m}\text{-xylene}) = 2.31 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Calvert et al., 2002).
- (b) Relative to HO + cyclohexane  
(c) Relative to HO + *m*-xylene

#### Preferred Values

Parameter	Value	$T/\text{K}$
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.45 \times 10^{-11}$	298
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.20$	298

#### Comments on Preferred Values

The preferred value is an average of the relative rate coefficients of Aschmann and Atkinson (1998) obtained with two reference compounds. In the presence of O<sub>2</sub>, the reaction of OH with 1,2-ethanediol is expected to produce glycolaldehyde (HOCH<sub>2</sub>CHO) with a formation yield of unity:



### References

- Aschmann, S. M., and Atkinson, R.: *Int. J. Chem. Kinet.*, 30, 533, 1998.
- Calvert, J. G., Atkinson, R., Becker, K. H., Kamens, R. M., Seinfeld, J. H., Wallington, T. J., and Yarwood, G.: *The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons*, Oxford University Press, New York, NY, 2002.
- Calvert, J. G., Derwent, R. G., Orlando, J. J., Tyndall, G. S., and Wallington, T. J.: *Mechanisms of Atmospheric Oxidation of Alkanes*, Oxford University Press, New York, NY, 2008.