IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC73

This data sheet last evaluated: June 2009.

HO + $CH_3CH(OH)CH_2OH$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(2.18 \pm 0.12) \times 10^{-11}$	296 ± 2	Aschmann and Atkinson, 1998	RR (a, b)
$(2.02 \pm 0.14) \times 10^{-11}$	296 ± 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_3ONO-NO-air + 1,2-propanediol + *m*-xylene + methyl vinyl ketone mixtures at wavelengths > 300 nm. The concentrations of $CH_3CH(OH)CH_2OH$, *m*-xylene and methyl vinyl ketone (the reference compounds) were measured by gas chromatography with flame ionization detection (GC-FID). The measured rate coefficient ratios of k(HO + $CH_3CH(OH)CH_2OH$)/k(HO + *m*-xylene) = 0.944 ± 0.053 and k(HO + $CH_3CH(OH)CH_2OH$)/k(HO + methyl vinyl ketone) = 1.01 ± 0.07 are placed on an absolute basis using k(HO + *m*-xylene) = 2.31×10^{-11} cm^3 molecule^{-1} s^{-1} at 296 K (Calvert et al., 2002) and k(HO + methyl vinyl ketone) = 2.0×10^{-11} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson et al., 2006).

(b) Relative to HO + *m*-xylene.

(c) Relative to HO + methyl vinyl ketone.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.1×10^{-11}	298
Reliability		
$\Delta \log k$	± 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. Based on the product studies for the OH reaction with other diols (Bethel et al., 2001; Magneron et al., 2003), it is expected that the reaction of OH with 1,2-

propanediol proceeds mainly by H-atom abstraction from the >CH(OH) or -CH_2OH group leading to formation of hydroxyacetone and 2-hydroxypropanal:

$$HO + CH_3CH(OH)CH_2OH \rightarrow H_2O + CH_3C(OH)CH_2OH$$
$$HO + CH_3CH(OH)CH_2OH \rightarrow H_2O + CH_3CH(OH)CHOH$$

and

$$CH_3C(OH)CH_2OH + O_2 \rightarrow CH_3C(O)CH_2OH + HO_2$$
$$CH_3CH(OH)CHOH + O_2 \rightarrow CH_3CH(OH)CHO + HO_2$$

References

Aschmann, S. M., and Atkinson, R.: Int. J. Chem. Kinet., 30, 533, 1998.

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.

Bethel, H. L., Atkinson, R., and Arey, J.: Int. J. Chem. Kinet., 33, 310, 2001.

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.

Magneron, I., Bossoutrot, V., Mellouki, A., Laverdet, G., and Le Bras, G.: Environ. Sci. Technol., 37, 4170, 2003.