IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC72

This data sheet last evaluated: June 2009.

HO + $CH_3CH(OH)CHO \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.7 \pm 0.2) \times 10^{-11}$	296 ± 2	Baker et al., 2004	RR-GC (a, b)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO-NO-air mixtures at 740 Torr total pressure of purified air at > 300 nm. Experiments were carried out in a 7500 liter Teflon chamber. 2-hydroxypropanal was generated in situ from the OH radical-initiated reaction of 2-methyl-3-buten-2-ol. The concentrations of 2-hydroxypropanal and its precursor, 2-methyl-3-buten-2-ol, were measured by gas chromatography. From comparison of the measured time-concentration behaviour of $CH_3CH(OH)CHO$ and its precursor with calculations, rate coefficient ratio of k(HO + 2-hydroxypropanal)/k(HO + 2-methyl-3-buten-2-ol) = 0.657 ± 0.050 was derived. This rate coefficient ratio is placed on an absolute basis by use of rate coefficients at 296 K k(HO + 2-methyl-3-buten-2-ol) = 6.0×10^{-11} cm^3 molecule^{-1} s^{-1}.

(b) Relative to HO + 2-methyl-3-buten-2-ol.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.7×10^{-11}	298
Reliability		
$\Delta \log k$	± 0.20	298

Comments on Preferred Value

The recommendation is based upon the relative study by Baker et al. (2004).

Based on the fact the rate coefficients for OH reaction with $CH_3CH(OH)CHO$ is similar to that with $HOCH_2CHO$ and $(CH_3)_2C(OH)CHO$, Baker et al. have suggested that the majority of reaction of OH with $CH_3CH(OH)CHO$ proceeds by H-atom abstraction from the CHO group, as is the case for $HOCH_2CHO$ (Atkinson et al., 2006).

References

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.
Baker, J, Arey, J. and Atkinson, R.: J. Phys. Chem. A, 108, 7032, 2004.