IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC67

This data sheet last evaluated: June 2009.

HO + *n*-$C_3H_7C(O)OH$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.8 \pm 0.16) \times 10^{-12}$	298	Zetzsch and Stuhl, 1982	FP-RF (a)

Comments

(a) HO radicals were generated by the vacuum ultraviolet ($\lambda \geq 105$ nm) photolysis of H_2O and monitored as function of time under pseudo-first order conditions by resonance fluorescence.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.8×10^{-12}	298
Reliability		
$\Delta \log k$	± 0.30	298

Comments on Preferred Values

The preferred rate coefficient value at 298 K is based on the sole study of Zetzsch and Stuhl (1982). This value is higher than those for the shorter chain organic acids ($CH_3C(O)OH$ and $C_2H_5C(O)OH$, respectively, $k = 7.4 \times 10^{-13}$ and 1.2×10^{-12} cm^3 molecule^{-1} s^{-1}, Atkinson et al., 2006).

As with the other acids, it is expected that the reaction will occur both at the acidic site (–C(O)OH) and the alkyl site (n-C_3H_7-).

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.

Zetzsch, C., and Stuhl, F.: (1982), *Physico-chemical behaviour of atmospheric pollutants*, edited by B. Versino and H. Ott, D. Reidel Publishing Company, Dordrecht, 129,1982.