IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx96; VII.A5.15

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$$HO + CF_3CH(OH)_2 \rightarrow CF_3C(OH)_2 + H_2O \quad (1)$$
$$\rightarrow CF_3CH(OH)O + H_2O \quad (2)$$

Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.18 \pm 0.11) \times 10^{-12}$	296	Andersen et al. (2006)	RR (a)
$(1.14 \pm 0.12) \times 10^{-12}$	296		

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO in 700 Torr (933 mbar) of air. Separate experiments were performed using C_2H_2 and C_2H_4 as references. Rate coefficient ratios of $k(HO+CF_3CH(OH)_2)/k(HO+C_2H_2) = 0.146 \pm 0.015$ and $k(HO+CF_3CH(OH)_2)/k(HO+C_2H_4) = 0.0149 \pm 0.0014$ were reported. Using $k(HO+C_2H_2) = 7.8 \times 10^{-13}$ and $k(HO+C_2H_2) = 7.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006) gives $k(HO+CF_3CH(OH)_2) = (1.14 \pm 0.12) \times 10^{-13}$ and $(1.18 \pm 0.11) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.2×10^{-13}	298
Reliability		
$\Delta \log k$	0.20	298

Comments on Preferred Values

The recommendation is based upon the average of the two determinations by Andersen et al. (2006). Andersen et al. (2006) reported that the chlorine atom initiated oxidation of $CF_3CH(OH)_2$ in 700 Torr (933 mbar) of air gives $CF_3C(O)OH$ in a molar yield of 101 ± 6%. The HO radical initiated of $CF_3CH(OH)_2$ is expected to give $CF_3C(O)OH$ in essentially 100% yield.

References

Andersen, M. P. S., Nielsen, O. J., Hurley, M. D., Ball, J. C., Wallington, T. J., Ellis, D. A., Martin, J. W., and Mabury, S. A.: J. Phys. Chem. A, 109, 1849, 2005.

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 Subcommittee for Gas Kinetic Data Evaluation, http://iupac.pole-ether.fr.