IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx85; VII.A5.2

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$$HO + CHF_2CH_2OH \rightarrow CF_2CH_2OH + H_2O \quad (1)$$
$$\rightarrow CHF_2CHOH + H_2O \quad (2)$$
$$\rightarrow CHF_2CH_2O + H_2O \quad (3)$$

Rate coefficient data ($k = k_1 + k_2 + k_3$)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.52 \pm 0.44) \times 10^{-13}$	300	Kovacs et al. (2005)	FP-RF (a)
Relative Rate Coefficients			
$(4.57 \pm 0.38) \times 10^{-13}$	298	Sellevåg et al. (2004)	RR (b)

Comments

(a) HO radicals were produced by the photolysis of HNO_3 at 248 nm in 105 ± 5 mbar of helium diluent.

(b) HO radicals were generated by the photolysis of O_3 in the presence of H_2O in 1013 mbar of air diluent at 298 K. A rate coefficient ratio of $k(HO+CHF_2CH_2OH)/k(HO+C_2H_6) = 1.903 \pm 0.016$ was measured. Placing this on an absolute basis using $k(HO+C_2H_6) = 2.4 \times 10^{-13}$ (Atkinson et al., 2006) gives $k(HO+CHF_2CH_2OH) = (4.57 \pm 0.38) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	3.6×10^{-13}	298
Reliability		
$\Delta \log k$	± 0.25	298

Comments on Preferred Values

There is a significant discrepancy between the rate coefficients at ambient temperature reported by Sellevåg et al. (2004) and Kovacs et al. (2005). There is no obvious reason to favor one study over the other and our recommended rate coefficient is the average of the two studies. Clearly further work to resolve this discrepancy is needed.

References

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Kovacs, G., Szasz-Vadasz, T., Papadimitriou, V. C., Dóbé, S., Bérces, T., and Marta F.: React. Kinet. Catal. Lett., 87, 129, 2005.

Sellevåg, S. R., Nielsen, C. J., Søvde, O. A., Myhre, G., Sundet, J. K., Stordal, F., and Isaksen, I. S. A.: Atmos. Environ., 38, 6725, 2004.