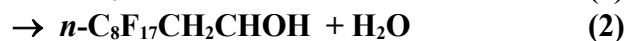


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet of O_x95; VII.A5.12

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The citation for the preferred values in this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

This datasheet last evaluated: June 2015; last change in preferred values: June 2009.



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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(9.2 \pm 1.2) \times 10^{-13}$	296	Ellis et al. (2003)	RR (a)

Comments

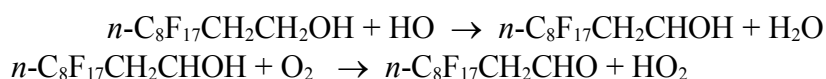
- (a) HO radicals were generated by the photolysis of CH₃ONO in 700 Torr (933 mbar) of air. Experiments were performed with *n*-C₄F₉CH₂CH₂OH, *n*-C₆F₁₃CH₂CH₂OH, and *n*-C₈F₁₇CH₂CH₂OH. There was no discernable difference in the reactivity of the three alcohols and the composite data set was analyzed together. A rate coefficient ratio of $k(\text{HO} + \text{C}_x\text{F}_{2x+1}\text{CH}_2\text{CH}_2\text{OH})/k(\text{HO} + \text{C}_2\text{H}_2) = 1.18 \pm 0.15$ was reported. Using $k(\text{HO} + \text{C}_2\text{H}_2) = 7.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006) gives $k(\text{HO} + n\text{-C}_8\text{F}_{17}\text{CH}_2\text{CH}_2\text{OH}) = (9.2 \pm 1.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	9.2×10^{-13}	298
<i>Reliability</i>		
$\Delta \log k$	0.15	298

Comments on Preferred Values

The rate coefficient reported by Ellis et al. (2003) is recommended. As discussed by Calvert et al. (2011), HO radicals are approximately an order of magnitude less reactive towards C_xF_{2x+1}CH₂OH than towards C_xF_{2x+1}CH₂CH₂OH and it seems likely that the majority (>90%) of reaction of HO with *n*-C₈F₁₇CH₂CH₂OH proceeds via attack on the terminal –CH₂– group. As with other α-hydroxy alkyl radicals, the atmospheric fate of *n*-C₈F₁₇CH₂CHOH radicals will be reaction with O₂ to give the corresponding aldehyde.



It is expected that the HO radical initiated oxidation of *n*-C₈F₁₇CH₂CH₂OH will lead to the formation of *n*-C₈F₁₇CH₂CHO in a yield of essentially 100%. Consistent with this expectation,

Chiappero et al. (2008) measured a $92 \pm 7\%$ yield of $n\text{-C}_8\text{F}_{17}\text{CH}_2\text{CHO}$ in the chlorine atom initiated oxidation of $n\text{-C}_8\text{F}_{17}\text{CH}_2\text{CH}_2\text{OH}$ (8:2 FTOH) in 700 Torr of air.

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 Subcommittee for Gas Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.
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- Chiappero, M. S., Argüello, G. A., Hurley, M. D., and Wallington, T. J.: *Chem. Phys. Lett.*, 461, 198, 2008.
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