# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx80; VII.A1.9



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.

**HO + $CF_3CH_2CF_2CH_2CF_3$ (HFC-458mfcf) → $CF_3CHCF_2CH_2CF_3$ + $H_2O$**

## Rate coefficient data (*k*)

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | $T$/K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $1.23 \times 10^{-13}$ exp[-1833/T] | 278-354 | Nelson et al. (1995) | FP-RF (a) |
| $(2.55 \pm 0.15) \times 10^{-15}$ | 298 | | |

## Comments

(a) HO radicals were produced by the reaction of H atoms with $NO_2$. Experiments were performed in 0.8-6.4 Torr (1.1-8.5 mbar) of helium diluent.

## Preferred Values

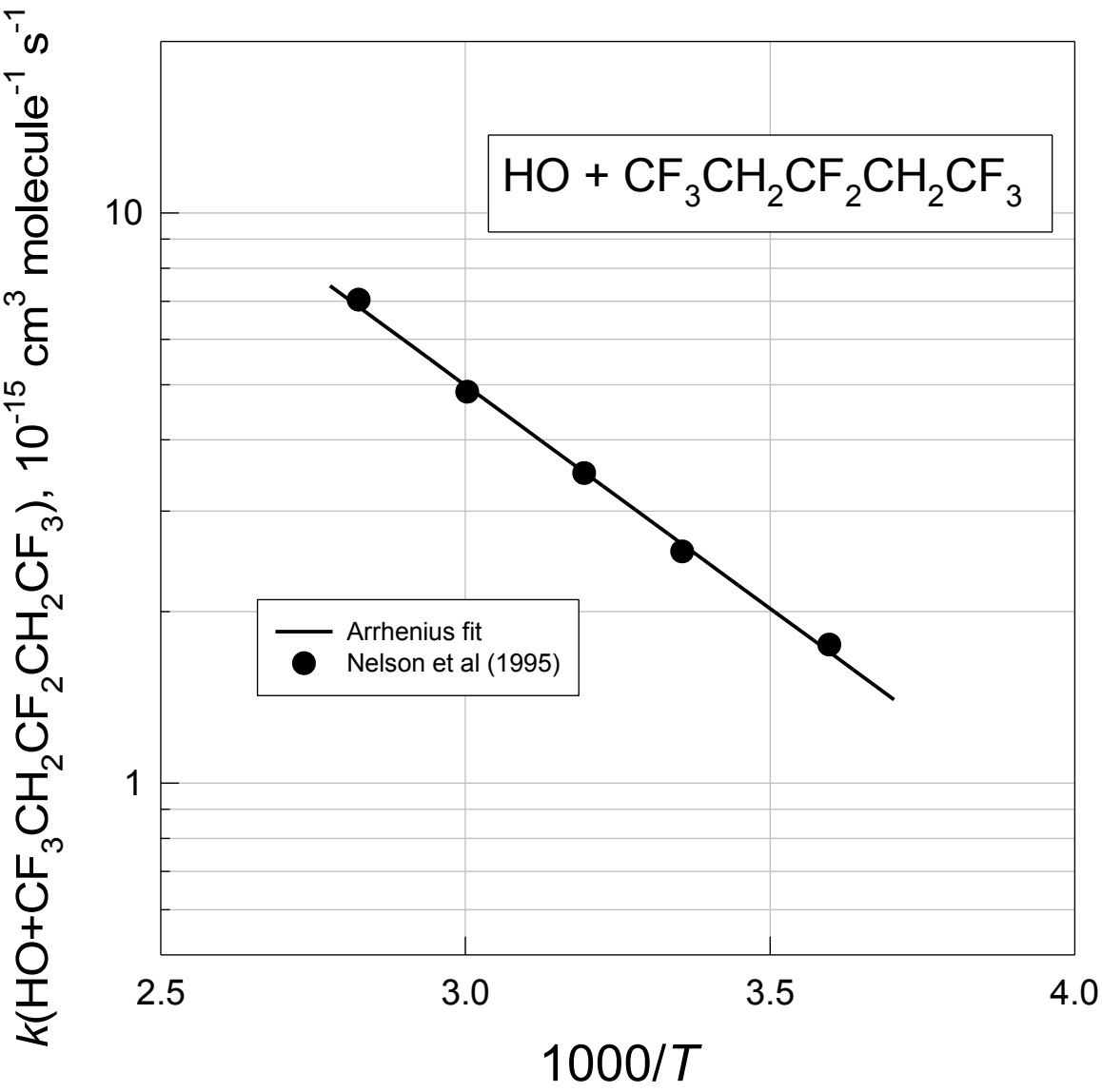
| Parameter | Value | $T$/K |
|---|---|---|
| $k$ | $2.6 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ | 298 |
| | $1.12 \times 10^{-12}$ exp(-1804/T) cm$^3$ molecule$^{-1}$ s$^{-1}$ | 270-360 |
| *Reliability* | | |
| $\Delta$ log $k$ | 0.15 | 298 |
| $\Delta$ E/R | ± 300 | 270-360 |

*Comments on Preferred Values*

A fit to the data from Nelson et al. (1995) gives $k$(HO+$CF_3CH_2CF_2CH_2CF_3$) = $1.12 \times 10^{-12}$ exp(-1804/T) cm$^3$ molecule$^{-1}$ s$^{-1}$ which is recommended. This expression gives $k$(HO+$CF_3CH_2CF_2CH_2CF_3$) = $2.6 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.

## References

Nelson Jr., D.D., Zahniser, M.S, Kolb, C.E, and Magid, H.: J. Phys. Chem., 99 16301, 1995.


HO + CF3CH2CF2CH2CF3
Arrhenius fit
Nelson et al (1995)
10
1
2.5
3.0
3.5
4.0
1000/T
k(HO+CF3CH2CF2CH2CF3), 10-15 cm3 molecule-1 s-1