IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oBrOx7

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$HO + CF_3CH_2Br$ (Halon 2301) $\rightarrow H_2O + CF_3CHBr$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$8.5 \times 10^{-13} \exp[-(1113 \pm 35)/T]$	298-460	Orkin and Khamaganov, 1993	DF-EPR
$(2.05 \pm 0.16) \times 10^{-14}$	298		
$1.39 \times 10^{-12} \exp[-(1350 \pm 195)/T]$	280-353	Nelson et al., 1993	DF-LIF
$(1.45 \pm 0.13) \times 10^{-14}$	294		

Preferred Values

$k = 1.6 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 1.4 \times 10^{-12} \exp(-1340/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 280-460 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.
$\Delta(E/R) = \pm 300$ K.

Comments on Preferred Values

The rate coefficients of Nelson et al. (1993) are ~15-25% lower than those of Orkin and Khamaganov (1993) over the temperature range common to both studies (298-353 K). A least-squares analysis of the rate coefficients of Orkin and Khamaganov (1993) and Nelson et al. (1993) yields the preferred Arrhenius expression.

References

Nelson Jr., D. D., Zahniser, M. S. and Kolb, C. E.: Geophys. Res. Lett. 20, 197, 1993.
Orkin, V. L. and Khamaganov, V. G.: J. Atmos. Chem. 16, 169, 1993.