# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oBrOx20; VII.A3.5



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$$HO + CH_3CHBrCH_3 \rightarrow CH_2CHBrCH_3 + H_2O \quad (1)$$
$$\rightarrow CH_3CBrCH_3 + H_2O \quad (2)$$

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

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | $T$/K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $(3.58\pm0.47) \times 10^{-12}$ exp[-(392±75)/T)] | 233-372 | Téton et al. (1996) | PLP-LIF (a) |
| $9.42 \times 10^{-13}$ | 298 | | |
| $7.0 \times 10^{-14}$ $T^{0.5}$ exp (-145/T) | 215-402 | Herndon et al. (2001) | PLP-LIF (b) |
| $(7.45\pm0.15) \times 10^{-13}$ | 298 | | |
| $1.66 \times 10^{-13}$ $(T/298)^{2.95}$ exp(461/T) | 210-480 | Kozlov et al. (2003) | FP-RF (c) |
| $(7.58\pm0.12) \times 10^{-13}$ | 298 | | |
| $1.56 \times 10^{-17}$ $T^{4.18}$ exp(922/T) | 297-715 | Bryukov et al. (2007) | PLP-LIF (d) |
| $7.53 \times 10^{-13}$ | 297 | | |
| *Relative Rate Coefficients* | | | |
| $(8.16 \pm 0.35) \times 10^{-13}$ | 298 | Donaghy et al. (1993) | RR (e) |

## Comments

(a) The value at 298 K is the average of the five determinations reported by Téton et al. (1996) at this temperature.
(b) HO radicals were produced by the photolysis of HONO at 355 nm (third harmonic Nd:YAG laser) in approximately 100 Torr (133 mbar) of helium diluent.
(c) HO radicals were generated by the photolysis of $H_2O$ using a xenon flash lamp. Experiments were performed in 30 Torr (4 mbar) of argon diluent.
(d) The value at 297 K is the average of the five determinations reported by Bryukov et al. (2003) at this temperature.
(e) The rate coefficient ratio $k$(HO+$C_3H_5Br$)/$k$(HO+cyclohexane) = 0.117 ± 0.005 was placed on an absolute basis using $k$(HO+cyclohexane) = $3.26 \times 10^{-17}$ $T^2$ exp(-262/$T$) cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson, 2003).

## Preferred Values

| Parameter | Value | $T$/K |
|---|---|---|
| $k$ /cm$^3$ molecule$^{-1}$ s$^{-1}$ | $7.58 \times 10^{-13}$ | 298 |
| $k$ /cm$^3$ molecule$^{-1}$ s$^{-1}$ | $1.96 \times 10^{-12}$ exp(-283/T) | 210-335 |
| *Reliability* | | |
| $\Delta \log k$ | 0.06 | 298 |
| $\Delta$ E/R | ± 200 | |

*Comments on Preferred Values*

The rate coefficients obtained in the absolute rate studies by Herndon et al. (2001), Kozlov et al. (2003), and Bryukov et al. (2003) and in the relative rate study by Donaghy et al. (1993) are in good agreement over the temperature ranges where comparison is possible. Results from the absolute rate study by Téton et al. (1996) lie in general approximately 20% above those from the other studies. The three parameter equation $k = CT^2 \exp(-D/T)$ is not able to capture the magnitude of the curvature evident in the Arrhenius plot. Fitting a double Arrhenius expression of $k = A \exp(-B/T) + C \exp(-D/T)$ to the composite data set (excluding the data from Téton et al. (1996)) gives $k = 1.07 \times 10^{-10} \exp(-2413/T) + 1.66 \times 10^{-12} \exp(-246/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ which provides a good description of the reported rate coefficients over the temperature range 210-720 K. For inclusion into atmospheric chemistry models we recommend the Arrhenius expression $k = 1.96 \times 10^{-12} \exp(-283/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ obtained by fitting the Arrhenius expression to the data from Donaghy et al. (1993), Herndon et al. (2001), Kozlov et al. (2003), and Bryukov et al. (2003) over the range 210-335 K.

## References


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Kozlov, S. N., Orkin, V. L., Huie, R. E., and Kurylo, M. J.: J. Phys. Chem. A, 107, 1333, 2003.

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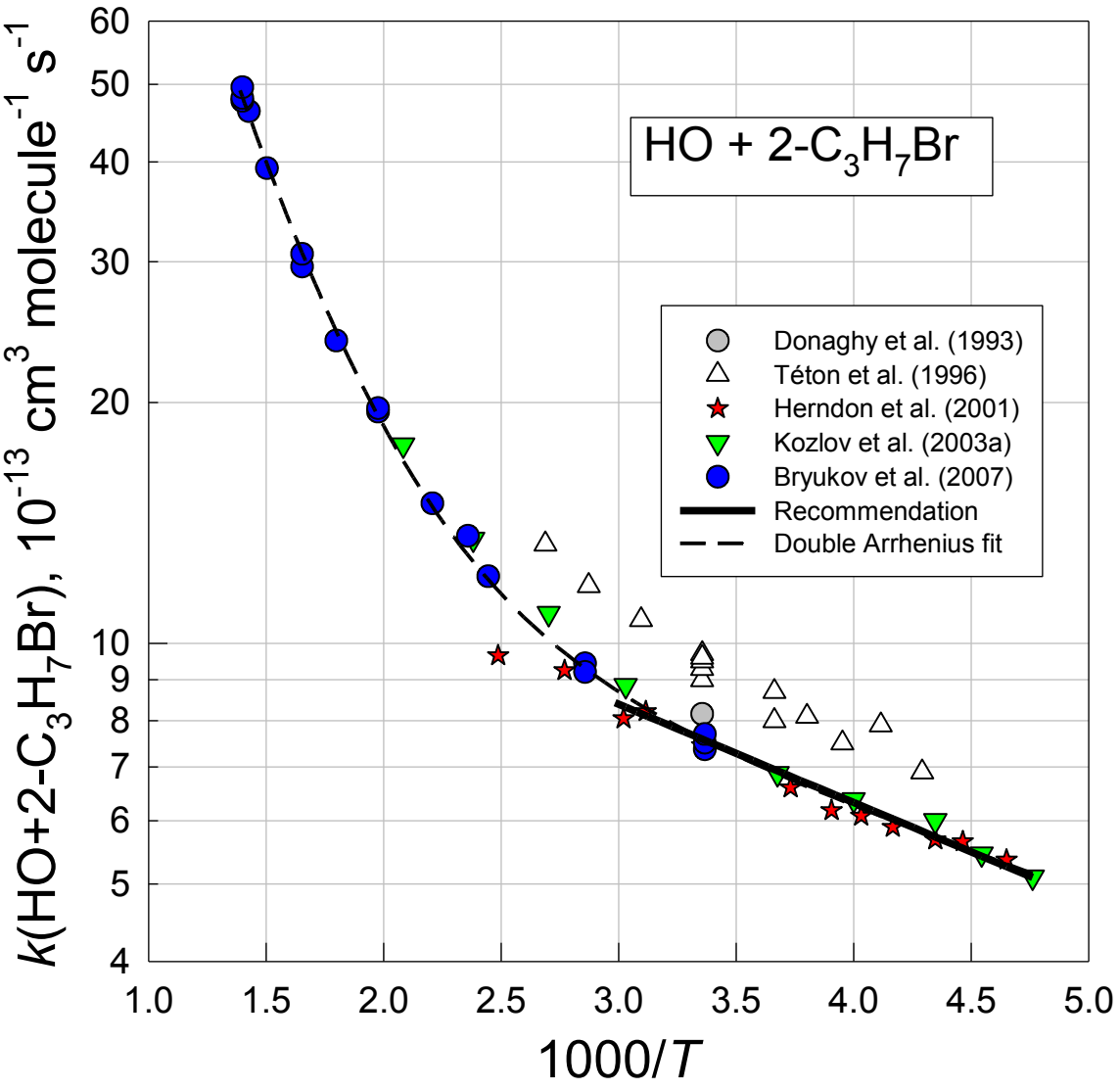
HO + 2-C3H7Br
Donaghy et al. (1993)
Téton et al. (1996)
Herndon et al. (2001)
Kozlov et al. (2003a)
Bryukov et al. (2007)
Recommendation
Double Arrhenius fit
k(HO+2-C3H7Br), 10-13 cm3 molecule-1 s-1
1000/T
60
50
40
30
20
10
9
8
7
6
5
4
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0