# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC79



This data sheet last evaluated: June 2011; last change in preferred values: June 2011.

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## $HO_2 + CH_3CH(OH)CH(O_2)CH_3 \rightarrow$ products

### Rate coefficient data

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients*<br>$(1.5 \pm 0.4) \times 10^{-11}$ | 296 | Jenkin and Hayman, 1995 | PLP-UVA (a) |

### Comments

(a) PLP-UV absorption study of $H_2O_2$-but-2-ene-$O_2$-$N_2$ mixtures at 1 bar (750 Torr) and 296 K. Conditions were chosen such that the initial $[HO_2]/[CH_3CH(OH)CH(O_2)CH_3]$ was varied in the range 0.7 – 7.1. $k$ was determined from simulation of transient decay traces recorded at 220 nm, 230 nm and 260 nm, with different relative contributions to the signals being due to $CH_3CH(OH)CH(O_2)CH_3$ and $HO_2$ absorption. No systematic dependence of the derived $k$ on initial $[HO_2]/[CH_3CH(OH)CH(O_2)CH_3]$ was observed.

### Preferred Values

| Parameter | Value | T/K |
|---|---|---|
| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | $1.5 \times 10^{-11}$ | 298 |
| *Reliability* | | |
| $\Delta \log k$ | $\pm 0.3$ | 298 |

*Comments on Preferred Values*

The preferred rate coefficient is based on the sole kinetics study of Jenkin and Hayman (1995). Although the value of $k$ is comparable with those reported for the reactions of $HO_2$ with other β–hydroxyalkyl peroxy radicals, $HOCH_2CH_2O_2$ (see datasheet HOx_VOC55) and $(CH_3)_2C(OH)C(O_2)(CH_3)_3$ (Boyd et al., 2003), confirmatory studies are required to reduce the recommended uncertainty limits.

By analogy with the reaction of $HO_2$ with $HOCH_2CH_2O_2$, it is likely that the reaction mainly yields $CH_3CH(OH)CH(OOH)CH_3$ and $O_2$. Indeed, the API-MS study of Tuazon et al. (1998) reported formation of this hydroxyhydroperoxide, during the HO initiated oxidation of *cis*-but-2-ene and *trans*-but-2-ene in the absence of $NO_x$ (at 297 K and 986 mbar), attributed to the reaction of $CH_3CH(OH)CH(O_2)CH_3$ with $HO_2$; although further product studies are required to quantify the branching ratio. Dillon and Crowley (2008) have investigated the

formation of HO from the reactions of $HO_2$ with selected $RO_2$ radicals. In the case of the structurally similar peroxy radicals, $HOCH_2CH_2O_2$ and $CH_3CH(OH)CH_2O_2$, respective upper limits of 0.04 and 0.06 were reported for the propagating channels forming HO, $O_2$ and the corresponding oxy radical. It is therefore probable that the title reaction is also mainly (or exclusively) terminating.

## References


Boyd, A. A., Flaud, P-M., Daugey, M. and Lesclaux, R.: J. Phys. Chem. A, 107, 818, 2003.
Dillon, T. J. and Crowley, J. N.: Atmos. Chem. Phys., 8, 4877, 2008.
Jenkin, M. E. and Hayman, G. D.: J. Chem. Soc. Faraday Trans., 91, 1911, 1995.
Tuazon, E.C., Aschmann, S.M., Arey, J. and Atkinson, R.: Environ. Sci. Technol., 32, 2106, 1998.