# Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC28

 This data sheet last evaluated: 2nd August 2007; no revision of preferred values.

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**HO + $CH_3CH(OH)CH_2CH_3$ → products**

## Rate coefficient data

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Relative Rate Coefficients* | | | |
| (8.58 ± 0.49) x $10^{-12}$ | 296 ± 2 | Chew and Atkinson, 1996 | RR (a) |
| (8.80 ± 0.14) x $10^{-12}$ | 297 ± 3 | Baxley and Wells, 1998 | RR (b,c) |
| (7.57 ± 0.44) x $10^{-12}$ | 297 ± 3 | Baxley and Wells, 1998 | RR (b,d) |

## Comments

(a) HO radicals were generated by the photolysis of $CH_3ONO$ in air, and the concentrations of 2-butanol and cyclohexane (the reference compound) were measured by GC. The measured rate coefficient ratio of $k$(HO + 2-butanol)/$k$(HO + cyclohexane) = 1.24 ± 0.07 is placed on an absolute basis by use of a rate coefficient of $k$(HO + cyclohexane) = 6.92 x $10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson, 2003).

(b) HO radicals were generated by the photolysis of $CH_3ONO$ in air, and the concentrations of 2-butanol and *n*-nonane and *n*-dodecane (the reference compounds) were measured by GC. The measured rate coefficient ratios of $k$(HO + 2-butanol)/$k$(HO + *n*-nonane) and $k$(HO + 2-butanol)/$k$(HO + *n*-dodecane) are placed on an absolute basis by use of rate coefficients at 297 K of $k$(HO + *n*-nonane) = 9.69 x $10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k$(HO + *n*-dodecane) = 1.32 x $10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson, 2003).

(c) Relative to HO + *n*-nonane.

(d) Relative to HO + *n*-dodecane.

## Preferred Values

$k$ = 8.7 x $10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.

*Reliability*

$\Delta \log k$ = ± 0.15 at 298 K.

*Comments on Preferred Values*

The preferred value is based on the relative rate coefficient of Chew and Atkinson (1996) and that of Baxley and Wells (1998) relative to HO + *n*-nonane, which are in excellent agreement.

The rate coefficient of Baxley and Wells (1998) measured relative to that for HO + *n*-dodecane, while in agreement with the other two rate coefficients (Chew and Atkinson, 1996; Baxley and Wells, 1998), is more uncertain because of the small data-base for HO + *n*-dodecane (Atkinson, 2003), and hence this rate coefficient is not used in the evaluation.

## References


Atkinson, R.: Atmos. Chem. Phys. 3, 2233, 2003.
Baxley, J. S. and Wells, J. R.: Int. J. Chem. Kinet. 30, 745, 1998.
Chew, A. A. and Atkinson, R.: J. Geophys. Res. 101, 28649, 1996.