

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_VOC73

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HO + CH₃CH(OH)CH₂OH → products

Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | T/K | Reference | Technique/ Comments |
|--|--------------|-----------------------------|---------------------|
| <i>Relative Rate Coefficients</i> | | | |
| $(2.18 \pm 0.12) \times 10^{-11}$ | 296 ± 2 | Aschmann and Atkinson, 1998 | RR (a, b) |
| $(2.02 \pm 0.14) \times 10^{-11}$ | 296 ± 2 | Aschmann and Atkinson, 1998 | RR (a, c) |

Comments

- (a) Relative rate method carried out at atmospheric pressure of air. HO radicals were generated by the photolysis of CH₃ONO-NO-air + 1,2-propanediol + *m*-xylene + methyl vinyl ketone mixtures at wavelengths > 300 nm. The concentrations of CH₃CH(OH)CH₂OH, *m*-xylene and methyl vinyl ketone (the reference compounds) were measured by gas chromatography with flame ionization detection (GC-FID). The measured rate coefficient ratios of $k(\text{HO} + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OH})/k(\text{HO} + m\text{-xylene}) = 0.944 \pm 0.053$ and $k(\text{HO} + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OH})/k(\text{HO} + \text{methyl vinyl ketone}) = 1.01 \pm 0.07$ are placed on an absolute basis using $k(\text{HO} + m\text{-xylene}) = 2.31 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Calvert et al., 2002) and $k(\text{HO} + \text{methyl vinyl ketone}) = 2.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al., 2006).
- (b) Relative to HO + *m*-xylene.
- (c) Relative to HO + methyl vinyl ketone.

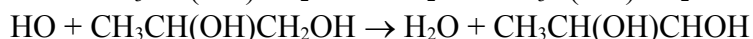
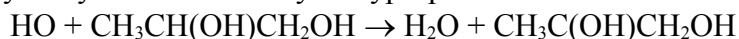
Preferred Values

| Parameter | Value | T/K |
|--|-----------------------|--------------|
| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | 2.1×10^{-11} | 298 |
| <i>Reliability</i> | | |
| $\Delta \log k$ | ± 0.20 | 298 |

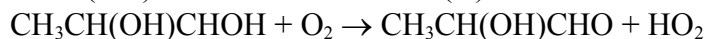
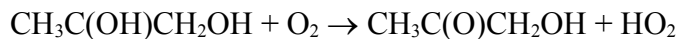
Comments on Preferred Values

The preferred value is an average of the relative rate coefficients of Aschmann and Atkinson (1998) obtained with two reference compounds. Based on the product studies for the OH reaction with other diols (Bethel et al., 2001; Magneron et al., 2003), it is expected that the reaction of OH with 1,2-

propanediol proceeds mainly by H-atom abstraction from the >CH(OH) or -CH₂OH group leading to formation of hydroxyacetone and 2-hydroxypropanal:



and



References

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