

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_AROM20

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HO + 3H-furan-2-one → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> $(4.87 \pm 0.29) \times 10^{-11}$	296 ± 2	Bierbach et al., 1994	RR-FTIR (a, b)

Comments

- (a) HO radicals were generated by the photolysis of H₂O₂ in 1000 mbar of air at $\lambda = 254$ nm. Experiments were carried out in a 1080-L quartz-glass chamber, and the concentrations of 3H-furan-2-one and propene (the reference compound) were measured in situ by long-path FTIR using an optical path length of 492 m and a spectral resolution of 1 cm⁻¹. The measured rate coefficient ratio of $k(\text{HO} + 3\text{H-furan-2-one})/k(\text{HO} + \text{propene}) = 1.68 \pm 0.10$ is placed on an absolute basis using $k(\text{HO} + \text{propene}) = 2.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006).
- (b) Relative to HO + propene.

Preferred Value

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	4.9×10^{-11}	298
<i>Reliability</i> $\Delta \log k$	± 0.20	298

Comments on Preferred Value

The preferred value is based on the sole study of Bierbach et al. (1994) in 1 bar of air but with higher uncertainty.

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

Bierbach, A., Barnes, I., Becker, K. H., and Wiesen, E.: Environ. Sci. Technol. 28, 715, 1994.