IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet NO3_VOC11 Website: <u>http://www.iupac-kinetic.ch.cam.ac.uk/</u>. See website for latest evaluated data. Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. This datasheet updated: 9th August 2002.

$NO_3 + CH_3C(O)CH_3 \rightarrow HNO_3 + CH_3C(O)CH_2$

 $\Delta H^{\circ} = -15.5 \text{ kJ} \cdot \text{mol}^{-1}$

Rate coefficient data

k/cm^3 molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $\leq (8.5 \pm 2.5) \ge 10^{-18}$	302	Boyd <i>et al.</i> , 1991 ¹	(a)

Comments

(a) Stopped flow system with detection of the NO₃ radical by optical absorption at 662 nm. Secondary reactions were believed to be important and a stoichiometry factor of ≥ 2 has been used to obtain the cited upper limit to the rate coefficient.

Preferred Values

 $k < 3 \ge 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$

Comments on Preferred Values

The upper limit to the preferred value is derived from the overall rate coefficient of $(1.7 \pm 0.5) \times 10^{-17} \text{ cm}^3$ molecule⁻¹ s⁻¹ measured by Boyd *et al.*,¹ with no account taken of the expected greater than unity stoichiometry.

References

¹ A. Boyd, C. E. Canosa-Mas, A. D. King, R. P. Wayne, and M. R. Wilson, J. Chem. Soc. Faraday Trans. **87**, 2913 (1991).