IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC13

This data sheet updated: 12th December 2007 (with no revision of the preferred values).

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

ΔH° = -15.5 kJ·mol^{-1}

Rate coefficient data

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

Comments

(a) Stopped flow system with detection of the NO_3 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

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

Comments on Preferred Values

The upper limit to the preferred value is derived from the overall rate coefficient of $(1.7 \pm 0.5) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} measured by Boyd et al. (1991), with no account taken of the expected greater than unity stoichiometry.

References

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