IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_4

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$2\text{-}C_3H_7O + O_2 \rightarrow CH_3COCH_3 + HO_2$

$\Delta H° = -150.3$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.51 \times 10^{-14} \exp[-(200 \pm 140/T)]$	294-384	Balla et al., 1985	PLP-LIF (a)
7.72×10^{-15}	298		
$1.4 \times 10^{-14} \exp[-(217 \pm 49)/T]$	218-311	Mund et al., 1998, 1999	PLP-LIF (b)
6.8×10^{-15}	298		
$1.6 \times 10^{-14} \exp[(-265 \pm 24)/T]$	288-364	Fittschen et al., 1999	PLP-LIF (c)
6.6×10^{-15}	298		
$1.6 \times 10^{-15} \exp[(492 \pm 568)/T]$	296-330	Deng et al., 2000	PLP-LIF (d)
8.2×10^{-15}	298		

Comments

(a) Pulsed laser photolysis of 2-propyl nitrite at 355 nm, with LIF detection of $2\text{-}C_3H_7O$ radicals. The pressure range was 1.3 mbar to 67 mbar (1 Torr to 50 Torr).

(b) Pulsed laser photolysis of propyl nitrite at 351 nm with laser-induced fluorescence detection of *i*-propoxy radical at 13 mbar total pressure of He. The individual rate coefficients at the various temperatures studied were not tabulated, but rather were presented only in graphical form.

(c) Pulsed laser photolysis of $2\text{-}C_3H_7ONO$ at 351 nm in $2\text{-}C_3H_7ONO\text{-}O_2$-He mixtures in the range 40-270 mbar (30-200 Torr) with LIF detection of $2\text{-}C_3H_7O$ excited at 347 nm and fluorescence detection to the red of 375 nm. The upper temperature limit is set by the unimolecular decomposition rate of *i*-propoxy radical. Combining their data with those of Mund et al. (1998, 1999) resulted in the Arrhenius expression $k = 1.9 \times 10^{-14} \exp[-(310 \pm 24)/T]$ cm^3 molecule^{-1} s^{-1} over the temperature range 218-364 K.

(d) Pulsed laser photolysis of 2-propyl nitrite at 355 nm with laser-induced fluorescence detection of *i*-propoxy radical. Their data could be equally well fit by the temperature independent expression $k = 7.6 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} over the narrow temperature range 296-333 K

Preferred Values

$k = 7.0 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K.

$k = 1.9 \times 10^{-14} \exp(-300/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 210-370 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.

$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The results of Balla et al. (1985), Mund et al. (1998, 1999) and Fittschen et al. (1999) are in excellent agreement. The preferred values are based on the temperature-dependent data of Mund et al. (1998, 1999) and Fittschen et al. (1999).

References

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Fittschen, C., Frenzel, A., Imrik, K., and Devolder, P.: Int. J. Chem. Kin. 31, 860, 1999.
Mund, Ch., Fockenberg, Ch., and Zellner, R.: Ber. Bunsenges. Phys. Chem. 102, 709, 1998.
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