IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A6.131 ROO_12

This datasheet last evaluated: June 2009. Last change in preferred values: June 2003.

$$C_2H_5O_2NO_2 + M \rightarrow C_2H_5O_2 + NO_2 + M$$

$\Delta H° = 67.7$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
4.8 x 10^{-4} exp(-9285/T) [N_2]	245-273	Zabel *et al*., 1989[1]	FTIR (a)

Comments

(a) Unimolecular decay of $C_2H_5O_2NO_2$ followed at total pressures ranging from 10 mbar to 800 mbar. Falloff extrapolation with $F_c = 0.3$.

Preferred Values

$k_0 = 1.4$ x 10^{-17} [N_2] s^{-1} at 298 K.
$k_0 = 4.8$ x 10^{-4} exp(-9285/T) [N_2] s^{-1} over the temperature range 250 K to 300 K.

Reliability

$\Delta \log k_0 = \pm 0.5$ at 298 K.
$\Delta (E/R) = \pm 1000$ K.

Comments on Preferred Values

The dissociation data are consistent with experimental recombination data from ref. 2 and the theoretical analysis from refs. 1 and 3. Falloff curves are constructed with $F_c = 0.31$ (over the range 250 K to 300 K).

High-pressure rate coefficients
Rate coefficient data

k_∞/s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			

$8.8 \times 10^{15} \exp(-10440/T)$	245-273	Zabel *et al*., 1989[1]	FTIR (a)

Comments

(a) See comment (a) for k_0.

Preferred Values

$k = 3.4\ s^{-1}$ at 298 K and 1 bar of air.
$k_\infty = 5.4\ s^{-1}$ at 298 K.
$k_\infty = 8.8 \times 10^{15} \exp(-10440/T)\ s^{-1}$, over the temperature range 250 K to 300 K.

Reliability

$\Delta \log k_\infty = \pm 0.5$ at 300 K.
$\Delta(E/R) = \pm 1000$ K.

Comments on Preferred Values

See comments on k_0.

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of k:

=((4.8e-4*exp(-9285/*T*))*M*(8.8e15*exp(-10440/*T*)))/((4.8e-4*exp(-9285/*T*))*M+(8.8e15*exp(-10440/*T*)))*10^(log10(0.31)/(1+(log10((4.8e-4*exp(-9285/*T*))*M/(8.8e15*exp(-10440/*T*)))/(0.75-1.27*log10(0.31)))^2))

The molecular density, $M = 7.243 \times 10^{21} P(bar)/T(K)$

References

1 F. Zabel, A. Reimer, K. H. Becker, and E. H. Fink, J. Phys. Chem. **93**, 5500 (1989).
2 G. Elfers, F. Zabel, and K. H. Becker, Chem. Phys. Lett. **168**, 14 (1990).
3 M. Destriau and J. Troe, Int. J. Chem. Kinet. **22**, 915 (1990).