IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A6.130 ROO_11

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

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

$\Delta H° = -67.7$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
4.8 x 10^{-29} [N_2]	254	Elfers, Zabel, and Becker, 1990[1]	(a)

Comments

(a) Thermal decomposition of $C_2H_5O_2NO_2$ in a glass reaction chamber in the presence of differing initial [NO_2]/NO] ratios at total pressures of 10 mbar to 1000 mbar. $C_2H_5O_2NO_2$ was prepared *in situ* by the photolysis of Cl_2-C_2H_6-O_2-NO_2-N_2 mixtures. $C_2H_5O_2NO_2$, NO_2 and NO concentrations were monitored by longpath FTIR absorption and rate coefficient ratios for the reaction of $C_2H_5O_2$ with NO and NO_2 were obtained. The reported rate coefficient for $C_2H_5O_2 + NO_2$ was derived using a rate coefficient of 8.9 x 10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction $C_2H_5O_2 + NO \rightarrow C_2H_5O + NO_2$. Falloff curves were constructed based on the theoretical analysis from ref. 2 with $F_c = 0.31$ and $k_\infty = 7.5 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

$k_0 = 1.3 \times 10^{-29} (T/300)^{-6.2}$ [N_2] cm^3 molecule^{-1} s^{-1} over the temperature range 200 K to 300 K.

Reliability

$\Delta \log k_0 = \pm 0.3$ at 298 K.

$\Delta n = \pm 1$.

Comments on Preferred Values

The preferred values are based on the data from ref. 1 and the analysis from ref. 2. The temperature dependence is from the theoretical analysis of ref. 2. Falloff extrapolations were made with $F_c = 0.31$ at 250 K to 300 K such as given from the theoretical analysis of ref. 2.

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Relative Rate Coefficients			
1.0 x 10^{-11}	254	Elfers, Zabel, and Becker, 1990[1]	(a)

Comments

(a) See comment (a) for k_0.

Preferred Values

k = 5.1 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K and 1 bar of air.
k_∞ = 8.8 x 10^{-12} cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 200 K to 300 K.

Reliability

$\Delta \log k_\infty = \pm 0.3$ over the temperature range 200 K to 300 K.

Comments on Preferred Values

See comments on k_0. The theoretical analysis in ref. 2 also includes information from studies of the reverse reaction measured in ref. 3.

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:

=((1.3e-29*(*T*/300)^-6.2)*M*(8.8e-12))/((1.3e-29*(*T*/300)^-6.2)*M+(8.8e-12))*10^(log10(0.31)/(1+(log10((1.3e-29*(*T*/300)^-6.2)*M/(8.8e-12))/(0.75-1.27*log10(0.31)))^2))

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

References

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