IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet R_Oxygen_5

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n-$C_3H_7 + O_2 + M \rightarrow n$-$C_3H_7O_2 + M$

High-pressure rate coefficients

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(5.5 \pm 0.9) \times 10^{-12}$	298	Ruiz and Bayes, 1984[1]	FP-MS (a)
6×10^{-12}	297	Slagle, Park and Gutman, 1985[2]	PLP-MS (b)

Comments

(a) No pressure dependence detected between 1.3 mbar and 5 mbar of He or N_2.

(b) n-C_3H_7 radicals were produced by CO_2 laser photolysis of $C_6F_7C_4H_9$. Only weak pressure dependences were observed over the range of He or N_2 pressures from 0.5 mbar to 9 mbar. The rate coefficient decreased from 6×10^{-12} cm^3 molecule^{-1} s^{-1} to 2.8×10^{-13} cm^3 molecule^{-1} s^{-1} over the temperature range 297 K to 635 K.

Preferred Values

$k = 6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K and 1 mbar to 10 mbar of air.

$k \approx k_\infty$ at 298 K and 1 bar of air.

$k_\infty = 8 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 200 K to 300 K.

Reliability

$\Delta \log k_\infty = \pm 0.2$ over the range 200 K to 300 K.

Comments on Preferred Values

The available experimental data are consistent with each other.[1,2] Because they were obtained at total pressures below 130 mbar, we estimate that some falloff corrections have to be applied and these are taken into account in the preferred values. These values are consistent with experiments for the reactions $C_2H_5 + O_2 + M \rightarrow C_2H_5O_2 + M$ and i-$C_3H_7 + O_2 + M \rightarrow i$-$C_3H_7O_2 + M$ (see this evaluation).

References

[1] R. P. Ruiz and K. D. Bayes, J. Phys. Chem. **88**, 2592 (1984).

[2] I. R. Slagle, J.-Y. Park, and D. Gutman, 20th Int. Symp. on Combustion 1984 (Combustion Institute, Pittsburgh, 1985), pp. 733-741.