IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_16

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$CH_3CH(O)CH_2CH_3 + NO \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$7.5 \times 10^{-12} \exp[(360 \pm 56)/T]$	226-311	Deng et al., 2000	PLP- LIF (a)
$(2.5 \pm 0.6) \times 10^{-11}$	298		
$9.1 \times 10^{-12} \exp[(409 \pm 72)/T]$	223-305	Lotz and Zellner, 2001	PLP-LIF (b)
$(3.6 \pm 0.3) \times 10^{-11}$	298		
$4.4 \times 10^{-12} \exp((590 \pm 36)/T)$	223-348	Falgayrac et al., 2004.	PLP-LIF (c)
$(3.2 \pm 0.4) \times 10^{-11}$	298		

Comments

(a) Pulsed laser photolysis at 351 nm of a mixture of 2-butylnitrite and NO at a total pressure of N_2 in the range 66.5 to 234 mbar in a slow flow reactor monitored by laser-excited fluorescence detection of 2-butoxy radical at 365.8 nm. No pressure dependence was observed at 223 K.

(b) Pulsed laser photolysis at 351 nm / LIF detection of 2-butylnitrite in the presence of NO at a total pressure of N_2 of 26 mbar. The rate constant at 295 K is independent of pressure in the range 6.5-104 mbar N_2.

(c) Pulsed laser photolysis of 2-butyl nitrite/NO in He at 351 nm coupled to LIF detection of 2-butoxy radical excited near 369 nm in a slow flow reactor in the pressure range 26 to 394 mbar. The NO addition and the thermal decomposition of 2-butoxy radical are competitive under pseudo first order conditions, yet no marked pressure dependence of k was observed across the pressure range used. The Arrhenius expression in the Table refers to the combined data of Lotz and Zellner (2001) and Falgayrac et al. (2004) over the combined temperature range 223 to 348 K as Falgayrac et al. (2004) do not provide an Arrhenius expression of their own data.

Preferred Values

$k = 4.4 \times 10^{-12} \exp(590/T)$ over the temperature range 223-348 K.
$k = 3.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.
$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The data of Lotz and Zellner (2001) and Falgayrac et al. (2004) are recommended owing to the good agreement of the individual rate constants over the combined temperature range. The recent direct measurement of Falgayrac et al. (2004) extends the temperature range to 348 K. The recommended tabulated Arrhenius expression includes the data of Lotz and Zellner (2001) and of Falgayrac et al. (2004).

References

Deng, W., Wang, Ch., Katz, D. R., Gawinski, G. R., Davis, A. J. and Dibble, T. S.: Chem. Phys. Lett. 330, 541, 2000.
Falgayrac, G., Caralp, F., Sokolowski-Gomez, N., Devolder, P. and Fittschen, C.: Phys. Chem. Chem. Phys. 6, 4127, 2004.
Lotz, C. and Zellner, R.: Phys. Chem. Chem. Phys. 3, 2607, 2001.