IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_19

This data sheet updated: 12th June 2003.

$$1\text{-}C_3H_7O + NO_2 + M \rightarrow 1\text{-}C_3H_7ONO_2 + M \quad (1)$$
$$1\text{-}C_3H_7O + NO_2 \rightarrow CH_3CH_2CHO + HONO \quad (2)$$

$\Delta H°(1) = -165.9$ kJ·mol^{-1}
$\Delta H°(2) = -258.7$ kJ·mol^{-1}

High-pressure rate coefficients

Rate coefficient data

$k_{\infty 1}$/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
$(3.6 \pm 0.4) \times 10^{-11}$	296	Mund, Fockenberg, and Zellner, 1998[1]	PLP-LIF (a)

Comments

(a) The rate coefficient was observed to be independent of total pressure over the range 6.7 mbar to 53 mbar of He.

Preferred Values

$k_{\infty 1} = 3.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k_{\infty 1} = \pm 0.3$ at 298 K.

Comments on Preferred Values

The preferred value is based on the sole study of Mund *et al.*[1] with expanded uncertainty limits. The rate coefficient is of a similar magnitude to other RO + NO_2 reactions (see data sheets in this evaluation for $CH_3O + NO_2$, $C_2H_5O + NO_2$ and 2-$C_3H_7O + NO_2$).

Although no statement on the branching ratio k_1/k_2 may be made on the basis of this work, it is expected that $k_1/k_2 < 0.2$ (Suppl. IV).

References

[1] C. Mund, Ch. Fockenberg, and R. Zellner, Ber. Bunsenges. Phys. Chem. **102**, 709 (1998).