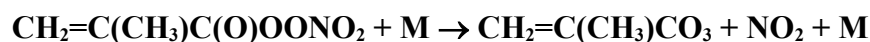


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet ROO_18

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This data sheet updated: 12th November 2002.



Rate coefficient data

k/s^{-1}	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.58 \times 10^{16} \exp[-(13488 \pm 504)/T]$ 3.5×10^{-4}	302.25-323.55 298*	Roberts and Bertman, 1992 ¹	(a)

Comments

- (a) The thermal decomposition of $\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{O})\text{OONO}_2$ (MPAN) was studied in one atmosphere of air, with added NO to ensure that $\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{O})\text{OO}$ radicals reacted with NO (to form $\text{NO}_2 + \text{CO}_2 + \text{CH}_2=\text{CCH}_3$) rather than reacting with NO_2 to reform MPAN. MPAN concentrations were measured by GC with electron capture detection.

Preferred Values

$k = 3.5 \times 10^{-4} \text{ s}^{-1}$ at 298 K and 1 bar.

$k = 1.6 \times 10^{16} \exp(-13500/T) \text{ s}^{-1}$ over the temperature range 290-330 K at 1 bar.

Reliability

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

$\Delta(E/R) = \pm 1000$ K.

Comments on Preferred Values

The preferred values are based on the sole study of this reaction by Roberts and Bertman.¹ The preferred values for the decomposition of MPAN are very similar to those for the thermal decomposition of $\text{CH}_3\text{C}(\text{O})\text{OONO}_2$ (PAN),^{1,2} and the rate coefficients measured by Roberts and Bertman¹ are expected, by analogy with the corresponding PAN decomposition,² to be very close to the high pressure limit at 1 bar of air.

References

¹ J. M. Roberts and S. B. Bertman, *Int. J. Chem. Kinet.* **24**, 297 (1992).

² IUPAC, <http://iupac.pole-ether.fr> (2013).