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

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This data sheet updated: 12th November 2002.

CH_2=C(CH_3)C(O)OONO_2 + M → CH_2=C(CH_3)CO_3 + NO_2 + M

Rate coefficient data

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

Comments

(a) The thermal decomposition of CH_2=C(CH_3)C(O)OONO_2 (MPAN) was studied in one atmosphere of air, with added NO to ensure that CH_2=C(CH_3)C(O)OO radicals reacted with NO (to form NO_2 + CO_2 + CH_2=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 x 10^{-4} s^{-1} at 298 K and 1 bar.
k = 1.6 x 10^{16} exp(-13500/T) s^{-1} over the temperature range 290-330 K at 1 bar.

Reliability

Δlog k = ±0.3 at 298 K.
Δ(E/R) = ±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 CH_3C(O)OONO_2 (PAN),[1,2] and the rate coefficients measured by Roberts and Bertman[1] 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).