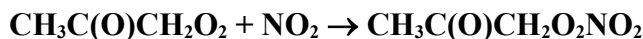


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet ROO_13

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: 24th November 2006.



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i> $(6.4 \pm 0.2) \times 10^{-12}$	295	Sehested et al., 1998	PR-AS (a)

Comments

- (a) Pulse radiolysis of a $\text{CH}_3\text{COCH}_3/\text{O}_2/\text{SF}_6/\text{NO}$ mixture at 1 atmosphere monitored by UV/VIS absorption of the peroxy radical at 310 nm and NO_2 . The rate constant was obtained by fitting to the transient absorption of NO_2 at 400 and 450 nm taking into account interfering reactions using chemical-kinetic simulation. The reverse first-order rate constant for decomposition of acetylperoxynitrate was measured in a static reactor monitored by FTIR absorption and resulted in $k_{-1} = 1.9 \times 10^{16} \exp(-10830/T) \text{ s}^{-1}$ resulting in $k_{-1} = 35^{-1}$ at 298 K.

Preferred Values

$k = (6.4 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K and 1 atm.

Reliability

$\Delta \log k = \pm 0.3$ at 295 K.

Comments on Preferred Values

The preferred values are based on the sole study of Sehested et al. (1998).

References

Sehested, J., Christensen, L. K., Nielsen, O. J., Bilde, M., Wallington, T. J., Schneider, W. F., Orlando, J. J. and Tyndall, G. S.: Int. J. Chem. Kin. 30, 475, 1998.