Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.
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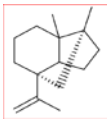
NO_3 +  (alloisolongifolene) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.41 \pm 0.24) \times 10^{-12}$	298 ± 2	Canosa-Mas et al., 1999	RR (a)

alloisolongifolene is: (4R,7aS)-1,7a-Dimethyl-4-(prop-1-en-2-yl)octahydro-1H-1,4-methanoindene.

Comments

(a) Relative rate of loss of alloisolongifolene and cyclohexa-1,4-diene (reference reactant) in a 56 L Teflon bag at 1013 mbar (760 Torr) of N_2 was monitored by GC-FID. NO_3 was generated by the thermal decomposition of N_2O_5. The rate constant ratio, $k(NO_3$ + alloisolongifolene) / $k(NO_3$ + cyclohexa-1,4-diene) = 2.14 ± 0.37 is placed on an absolute basis using $k(NO_3$ + cyclohexa-1,4-diene) = 6.6×10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson and Arey, 2003).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.4×10^{-12}	298
Reliability		
$\Delta \log k$	± 0.25	298

Comments on Preferred Values

The preferred value at 298 K is based on the relative rate study of Canosa-Mas et al. (1999). The error limits have been expanded to reflect the fact that this is the only study available.

There are no studies of the gas-phase products of this reaction, though it is expected to proceed predominantly via addition of NO_3 across the double bond to form a nitrooxyalkyl radical which can react with O_2 to form a nitrooxyalkyl peroxy radical.

References

Atkinson, R., and Arey, J., Chem. Rev., 103, 4605-4638, 2003.
Canosa-Mas, C. E., King, M. D., Scarr, P. J., Thompson, K. C., and Wayne, R. P., Phys. Chem. Chem. Phys., 1, 2929-2933, 1999.