

Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_VOC39

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Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$< 6 \times 10^{-18}$	296 ± 2	Shu and Atkinson, 1994	RR-GC (a),(b)
$< 5 \times 10^{-19}$	296 ± 2	Shu and Atkinson, 1994	RR-GC (a),(c)

longifolene is (1R,2S,7S,9S)-3,3,7-trimethyl-8-methylenetricyclo[5.4.0.0^{2,9}]undecane

Comments

- The concentrations of longifolene and *cis*-but-2-ene or propene (the reference compounds), with cyclohexane to scavenge HO radicals, were monitored by GC-FID in 6400–6900 L all Teflon chambers at 740 Torr (990 mbar) pressure of purified air in the presence of O₃. The measured coefficient ratios, $k(\text{O}_3 + \text{longifolene})/k(\text{O}_3 + \text{cis-but-2-ene})$ and $k(\text{O}_3 + \text{longifolene})/k(\text{O}_3 + \text{propene}) < 0.05$, are placed on an absolute basis using $k(\text{O}_3 + \text{cis-but-2-ene}) = 1.27 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k(\text{O}_3 + \text{propene}) = 1.01 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation) at 296 K.
- Relative to *cis*-but-2-ene.
- Relative to propene.

Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$< 5 \times 10^{-19}$	298

Comments on Preferred Values

The more stringent upper limit for the value of k reported in the study of Shu and Atkinson (1994) is adopted for the preferred value. This is based on no quantifiable decay of longifolene occurring in mixtures with O₃ and propene (with cyclohexane to scavenge HO radicals), for up to 75 % decay in the propene concentration. The low value of k compared to those for other terpenes possessing methylene groups (e.g. β -pinene and sabinene) is most likely due to steric hindrance resulting from the bridged ring structure.

References

Shu, Y. and Atkinson, R.: *Int. J. Chem. Kinet.*, 26, 1193, 1994.