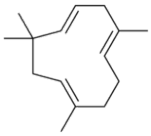
IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HOx_VOC93

This datasheet last evaluated: June 2014; last change in preferred values: June 2014.

OH +  **(α-humulene) → products**

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Relative Rate Coefficients			
$(2.9^{+0.7}_{-1}) \times 10^{-10}$	296±2	Shu and Atkinson, 1995	RR (a)

α-Humulene is 2,6,6,9-Tetramethyl-1,4-8-cycloundecatriene

Comments

(a) 6400 L Teflon chamber at 987 mbar (740 Torr) of air. OH radical was generated by the photolysis of CH_3ONO at wavelengths > 300 nm. α-Humulene and 2,3-dimethyl-2-butene (reference reactant) were monitored by GC-FID. The rate constant ratio, k(OH + α-humulene) / k(OH + 2,3-dimethyl-2-butene) = 2.66 ± 0.27 is placed on an absolute basis using k(OH + 2,3-dimethyl-2-butene) = 1.1×10^{-10} 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}	2.9 x 10^{-10}	298
Reliability		
Δ log k	0.10	298

Comments on Preferred Values

The preferred value of the rate coefficient at 298 K is based on the relative rate coefficient determination of Shu and Atkinson (1995). The reaction is expected to proceed predominantly by addition to the >C=C< double bonds.

References

Atkinson, R., and Arey, J.: Chem. Rev., 103, 4605-4638, 2003.
Shu, Y., and Atkinson, R.: J. Geophys. Res., 100, 7275-7281, 1995.