IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC31

This data sheet updated: 10th December 2007 (with no revision of the preferred values).

HO + 3-methylfuran → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients (9.26 ± 0.24) x 10^{-11}	296 ± 2	Atkinson et al., 1989	RR (a)

Comments

(a) Carried out at atmospheric pressure of air. HO radicals were generated by the photolysis of methyl nitrite-NO-air mixtures, and the concentrations of 3-methylfuran and 2,3-dimethyl-2-butene (the reference compound) were measured by GC. The measured rate coefficient ratio of k(HO + 3-methylfuran)/k(HO + 2,3-dimethyl-2-butene) = 0.842 ± 0.021 is placed on an absolute basis by use of a rate coefficient of k(HO + 2,3-dimethyl-2-butene) = 1.10 x 10^{-10} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson, 1997).

Preferred Values

k = 9.3 x 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

Δlog k = ±0.3 at 298 K.

Comments on Preferred Values

The preferred value is based on the sole study of this reaction by Atkinson et al. (1989). The reaction of HO radicals with 3-methylfuran is expected to proceed almost exclusively by initial HO radical addition to the C=C bonds (Atkinson et al., 1989).

References

Atkinson, R.: J. Phys. Chem. Ref. Data, 26, 215, 1997.

Atkinson, R., Aschmann, S. M., Tuazon, E. C., Arey, J. and Zielinska, B.: Int. J. Chem. Kinet., 21, 593, 1989.