IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM17

This data sheet last evaluated August 2008; last change in preferred values August 2008.

HO + 3-nitrotoluene → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.22 \pm 0.82) \times 10^{-12}$	298 ± 2	Atkinson et al., 1989	RR (a)

Comments

(a) HO radicals generated by the photolysis of CH_3ONO in air at atmospheric pressure in a ~6400 L Teflon chamber, with analyses of 3-nitrotoluene and benzene (the reference compound) by GC. The measured rate coefficient ratio k(HO + nitrobenzene)/k(HO + benzene) = 1.02 ± 0.68 is placed on an absolute basis using a rate coefficient of k(HO + benzene) = 1.2×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (IUPAC, current recommendation).

Preferred Values

$k = 1.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.5$ at 298 K.

Comments on Preferred Values

The preferred 298 K rate coefficient is based on the sole study reported to date.

References

Atkinson, R., Aschmann, S. M., Arey, J. and Carter, W. P. L.: Int. J. Chem. Kinet., 21, 801, 1989.
IUPAC: http://iupac.pole-ether.fr (2013).