IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC22

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

$NO_3 + C_2H_5OH \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$\leq$ 9 x 10^{-16}	298 ± 2	Wallington et al., 1987	FP-A
6.99 x 10^{-13} exp [-(1815 ± 419)/T]	273-367	Langer and Ljungström, 1995	DF-A
(1.81 ± 0.26) x 10^{-15}	297		

Preferred Values

k <2 x 10^{-15} cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

By analogy with the data for the reaction of the NO_3 radical with 2-propanol, it is likely that the rate coefficients of Langer and Ljungström (1995) are high because of the occurrence of secondary reactions. The preferred value is based on the upper limit to the rate coefficient determined by Wallington et al. (1987), and is consistent with the 298 K rate coefficient of Langer and Ljungström (1995) calculated from their Arrhenius expression. No recommendation is made concerning the temperature dependence.

References

Langer, S. and Ljungström, E.: J. Chem. Soc. Faraday Trans., 91, 405, 1995.
Wallington, T.J., Atkinson, R., Winer, A. M. and Pitts Jr., J. N.: Int. J. Chem. Kinet., 19, 243, 1987.