

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC25

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Cl + *i*-C₃H₇ONO₂ → products

Rate coefficient data

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> (3.8 ± 1.1) × 10 ⁻¹²	295 ± 2	Wallington et al., 1990	RR (a)

Comments

- (a) Cl atoms were generated by the photolysis of Cl₂ in Cl₂-isopropyl nitrate-C₂H₅Cl-air mixtures at 1 bar pressure. Concentrations of isopropyl nitrate and C₂H₅Cl were measured by GC, and a rate coefficient ratio of $k(\text{Cl} + \text{isopropyl nitrate}) / k(\text{Cl} + \text{C}_2\text{H}_5\text{Cl}) = 0.49 \pm 0.06$ determined. Rate coefficient in table calculated using $k(\text{Cl} + \text{C}_2\text{H}_5\text{Cl}) = 7.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Wine et al., 1983 and Bryukov et al., 2003).

Preferred Values

$$k = 3.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.3 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred 298 K rate coefficient is based on the sole study of Wallington *et al.* (1990).

References

- Bryukov, M. G., Slagle, I. R., and Knyazev, V. D.: J. Phys. Chem. A 107, 6565, 2003.
Wallington, T. J., Hinman, M. M., Andino, J. M., Siegl, W. O., and Japar, S. M.: Int. J. Chem. Kinet. 22, 665, 1990.
Wine, P. H., and Semmes, D. H.: J. Phys. Chem. 87, 3572, 1983.