IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_62

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**H2O + CH3CH2CHO (aq) → CH3CH2CH(OH)2 (aq)(1)**

**HO (aq) + CH3CH2CHO (aq) → products (2)**

**HO (aq) + CH3CH2CH(OH)2 (aq) → products (3)**

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Absolute Rate Coefficients* |
| (2.8 ± 0.3)  109 | 298 | 6.1 | - | Hesper, 2003 | LP-LPA (a) |
| 2.6  1011 exp[-(1300 ± 300)/T] | 283 - 313 | 6.1 | - |  |  |
| *Relative Rate Coefficients* |
| (2.33 ± 0.06)  109 | 298 | 5.2 | - | Mezyk, 1994 | PR / UV-Vis (b) |
| 8.01  1013 exp[-(3100 ± 100)/T] | 275 - 310 | 5.2 | - |  | PR / UV-Vis (b) |
| (3.65 ± 0.5)  109 | 298 | 2 | - | Monod et al., 2005 | Fenton reaction (c) |

The equilibrium constant for the hydration (1) is recommended as K298 K = 0.85 by Doussin and Monod (2013).

*GR* (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data *R* (g) are not available.

**Comments**

(a) Direct observation of the peroxyl-radicals at 248 nm, formed by the reaction between HO, propanal and O2. Reviewed by Herrmann (2003).

(b) Reference reaction: HO + SCN‑ with *k*(HO + SCN‑) = 1.22  1010 M‑1s‑1 according to Chin and Wine (1992); recalculation has been performed using the selected T dependence for the reference reaction by Zhu et al. (2003); experiments were performed in deoxygenated N2O / N2 saturated solutions.

(c) Radicals generated by dark Fenton reaction; Global rate constant for the reaction of HO radicals with propanal (2) and its hydrate (3) has been determined; K298 K was considered to be 0.71 (Bell and Evans, 1966); no specific information given on the reference reactions used for the determination; in general, multiple references were used: HO + methanol; *k*(T) = 9.7  108 exp[-4800/R(1/T-1/298)] (Elliot and Simsons, 1984); HO + 2-propanol; *k*(T) = 1.6  109 exp[-5000/R(1/T-1/298)] (Elliot and Simsons, 1984); HO + formaldehyde; *k*(T) = exp[-1020±90 (1/T)] (Chin and Wine, 1994).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 2.53  109 | 298 |
|  |  |  |
| *k* / L mol-1 s-1 | 8.25 × 1012 exp [-(2400)/T] | 275 - 313 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.24 | 298 |
| Δ EA/R | ±400 | 275 – 313 |
|  |  |  |

*Comments on Preferred Values*

Data from Mezyk (1994) and Hesper (2003) were used for regression. The rate coefficient determined by Monod et al. (2005) could not be used for further evaluation, as the publication does not identify the specific reference reactions. It is assumed that the value given results from a mean of determinations versus several reference systems. It is therefore not included in the regression for the determination of the preferred value. The estimated uncertainty of the recommended rate coefficient is given as Δ log *k* = ±0.24 or ±50%

**References**

Bell, R. P. and Evans, P. G.: Proc. R. Soc. Lond., Ser. A, 291(1426), 297-323, 1966.

Chin, M., and Wine, P. H: J. Photochem. Photobiol., A, 69(1), 17-25, 1992.

Doussin, J. F. and Monod, A.: Atmos. Chem. Phys., 13(23), 11625-11641, 2013.

Herrmann, H.: Chem. Rev., 103(12), 4691-4716, 2003.

Hesper, J.: Ph.D. Dissertation, University of Leipzig, Leipzig, Germany, 2003.

Mezyk, S. P.: Can. J. Chem., 72(4), 1116-1119, 1994.

Monod, A., Poulain, L., Grubert, S., Voisin, D. and Wortham, H.: Atmos. Env., 39(40), 7667-7688, 2005.

Zhu, L., Nicovich, J. M. and Wine, P. H.: Aquat. Sci., 65(4), 425-435, 2003.



T-dependent rate coefficients for the reaction of 1-propanal with HO in aqueous solution. Data from Mezyk (1994) and Hesper (2003) have been used for regression.