IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_66

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**H2O + CH3CH(CH2)2CHO (aq) → CH3CH(CH2)2CH(OH)2 (aq)(1)**

**HO (aq) + CH3CH(CH2)2CHO (aq) → products (2)**

**HO (aq) + CH3CH(CH2)2CH(OH)2 (aq) → products (3)**

**Rate coefficient data**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | |
| 3.0  109 | 294 | 2 | - | Acero et al., 2001 | Competition cinetics / HPLC (a) |

The equilibrium constant for the hydration (1) is recommended as K298 K = 0.23 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) HO radicals were generated by addition of O3 (2 × 10‑5 M) to an aqueous H2O2 (0.1 mM) solution; products analyzed by HPLC; Reference reaction: HO + pCBA with *k*(HO + pCBA) = 5  109M‑1s‑1 (Buxton et al., 1988); the rate coefficient has been recalculated using the recommended value for the reference reaction *k* = 4.64  109M‑1s‑1; *c*(2,2-dimethylpropanal) = 10‑3 M, *c*(pCBA) = 10 µM; Indigo method, as described by Bader and Hoigné (1981) was used for analyzing dissolved ozone; as no exact temperature is given, T = 294 K is assumed for room temperature.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 3.0  109 | 294 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.15 | 294 |

*Comments on Preferred Values*

The rate coefficient determined by Acero et al. (2003) is the only one available so far. Therefore, it is suggested to follow this value. The uncertainty of this determination is estimated as ±33% or Δ log *k* = 0.15. It should be noted that this rate coefficient refers to room temperature, which we estimate as T = 294 K.

**References**

Acero, J. L., Haderlein, S. B., Schmidt, T. C., Suter, M. J. F. and von Gunten, U.: Environ. Sci. Technol., 35(21), 4252-4259, 2001.

Bader, H. and Hoigné, J.: Water Res., 15(4), 449-456, 1981.

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