IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_82

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**H2O + CH3(CH2)2COCH3(aq) → CH3(CH2)2C(OH)2CH3(aq) (1)**

**HO(aq) + CH3(CH2)2COCH3(aq) → products (2)**

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 1.92  109 | 294 | 6 – 7 | - | Adams et al., 1965 | PR/ UV-Vis (a) |

The equilibrium constant for the hydration (1) has been estimated to be K298 K = 3.8 × 10-3 by Raventos-Duran et al. (2010).

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

**Comments**

(a) Reference reaction: HO + SCN- with *k*(HO + SCN-) = 6.6  109 M‑1s‑1; for the recalculation of the rate coefficient, the selected value for the reference reaction *k* = 1.10 × 1010 M‑1s‑1 was used; No exact value is given for the initial concentrations of the reactants; 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 | 1.92 × 109 | 294 |
|  |  |  |

*Reliability*

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

*Comments on Preferred Values*

The only determined rate constant for the aqueous phase oxidation of 2-pentanone by HO is the one of Adams et al. (1965). This rate constant has been recalculated, using the newly recommended rate constant for the reference reaction. The uncertainty of the recommended value 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**

Adams, G.E.; Boag, J.W.; Currant, J.; Michael, B.D., Pulse Radiolysis, Ebert, M.; Keene, J.P.; Swallow, A.J.; Baxendale, J.H. (eds.): Academic Press, New York, p.131-43, 1965.

Buxton, G. V., Greenstock, C. L., Helman, W. P., Ross, A. B.: J. Phys. Chem. Ref. Data, Vol. 12 (2), 513 – 886, 1988.

Raventos-Duran, T., Camredon, M., Valorso, R., Mouchel-Vallon, C. and Aumont, B.: Atmos. Chem. Phys., 10(16), 7643-7654, 2010.