IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_83

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This datasheet last evaluated: November 2019; last change in preferred values: June 2019

**H2O + CH3CH2CO CH2CH3 → CH3CH2C(OH)2CH2CH3 (1)**

**HO(aq) + CH3CH2COCH2CH3(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* | | | | | | |
| 1.35  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 | 1.35 × 109 | 294 |
|  |  |  |

*Reliability*

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

*Comments on Preferred Values*

The only determined rate constant for the oxidation of 3-pentanon is the one by Adams et al. (1965). This rate constant has been recalculated, using the newly recommended reference rate constant. The uncertainty of the recommendation 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.

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