IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_82

Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.   
The citation for this datasheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, [http://iupac.pole-ether.fr](http://iupac.pole-ether.fr/).

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

**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.