IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_11

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

HO (aq) + CH3CH2C(CH3)2OH (aq) → products

**Rate coefficient data**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| k/ l mol-1 s-1 | T/K | pH | | I/ mol l-1 | Reference | | | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | | | |
| 1.9 × 109 | 294 | 9 | - | | | Anbar et al.,  1966 | CW-radiolysis /UV-vis (a) | |

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

**Comments**

1. Reference reaction: HO + PNDA (p-nitrosodimethylaniline); the reference rate constant was determined versus ethanol with *k*(HO + ethanol) = 1.88 × 109 M‑1s‑1; no values given for initial concentrations; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than ±10%; 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 | 1.9 × 109 | 294 |
|  |  |  |

*Reliability*

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

*Comments on Preferred Values*

The former value recommended by Buxton et al. (1988) is also recommended. There have been no more recent determinations. The relative error of the rate constant is estimated as ±33% or Δ log*k* = ±0.15. It should be noted that this rate constant refers to room temperature, which we estimate as T = 294 K.

**References**

Anbar, M., Meyerstein, D. and Neta, P.: J. Chem. Soc. B, 742-747, 1966.

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