IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_50

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

**HO (aq) + HOC(CH3)2C(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* | | | | | | |
| 5.5  108 | 294 | 9 | - | Anbar et al., 1966 | PR / UV-Vis (a) |

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

**Comments**

(a) Reference reaction: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + PNDA (p-nitrosodimethylaniline); the reference rate constant was determined versus ethanol with *k*(HO + ethanol) = 1.10 × 109 M‑1s‑1; the recalculation of the rate coefficient was performed using the selected value for the reference reaction (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 temperature is given, for room temperature T = 294 K is assumed.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 5.47 × 108 | 298 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.15 | 298 |

*Comments on Preferred Values*

The only available rate constant determined by Adams et al. (1965), has been recalculated using the recommended rate constant for the reference reaction. The uncertainty of the recommended value is estimated to ±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**

Anbar, M., D. Meyerstein, and P. Neta: Journal of the Chemical Society B: Physical Organic, 742-747, 1966.