IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_45

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

**HO(aq) + CH3CH2CHOHCH2OH(aq) → products**

**Rate coefficient data**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | |
| (2.2 ± 0.4) × 109 | 298 | 7 | - | Hoffmann et al., 2009 | LFP-LPA (a) |
| 2.36 × 1011 exp[-(1400 ± 250)/T] | 288 - 328 | 7 | - |  | LFP-LPA (a1) |

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

**Comments**

(a) Radicals generated by laser flash photolysis (LFP) of H2O2 (*c*(H2O2) = 1  10-4 M) at 248 nm; rate constant was determined to be *k* = 2.3 × 109 M‑1s‑1, referring to reference reaction: HO + SCN- with *k*(HO + SCN-) = 1.24 × 1010 M‑1 s‑1; the selected temperature dependence by Zhu et al. (2003) was used for recalculation; *c*(KSCN) = 1.59  10-5 M. Arrhenius expression (a1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 2.2 × 109 | 298 |
|  |  |  |
| *k* / L mol-1 s-1 | 2.36 × 1011 exp[-(1400)/T] | 288 – 328 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.15 | 298 |
| Δ EA/R | ±250 | 288 – 328 |
|  |  |  |

*Comments on Preferred Values*

The rate constants determined by Hoffmann et al. (2009) are the only ones available for the reaction of butan-1,2-diol. They have been recalculated using the recommended rate constants for the reference reaction (Zhu et al., 2003). The uncertainty is estimated to be ±20 % or Δ log *k* = ±0.15.

**References**

Hoffmann, D., Weigert, B., Barzaghi, P. and Herrmann, H.: Phys. Chem. Chem. Phys., 11, 9351-9363, 2009.

Zhu, L., Nicovich, J. M. and Wine, P. H.: Aquat. Sci., 65(4), 425-435, 2003.

# plot 45 V1T-dependent rate constants for the reaction of butane-1,2-diol with HO in aqueous solution. Data from Hoffmann et al. (2009).