IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_10

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HO(aq) + C2H5CH(OH)C2H5(aq) → C2H5C(O)C2H5(aq) (45 -62%) + H2O + products

(Product distribution given by Snooke and Hamilton, 1974)

**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 | 1.7 - 1.8 | - | Snooke and Hamilton, 1974 | Fenton reaction/GC-FID (a) |

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

**Comments**

1. Cycloheptanol was used as a competing reagent; rate coefficient given as *k(*HO + 3-Pentanol)/*k*(HO + 2-Propanol) = 1.1; *k*(HO + 2-Propanol) has been used as k =1.1 – 1.7 × 109 M‑1s‑1, for the re-calculation here, *k* = (2.11 × 109 M‑1s‑1) has been used as the recommended reference reaction rate constant; *c*(FeSO4) = 3 × 10-3 mol/L, *c*(K2S2O8) = 3 × 10-3 mol/L, *c*(3-pentanol) given as ≥0.02 M; 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 only available determination by Snooke and Hamilton (1974) has been re-calculated with the recommended rate coefficient for the reference reaction. The change of the reference rate constants leads to a rate constant slightly smaller than the former recommendation by Buxton et al. (1988). . The estimated uncertainty of ±33% or Δ log *k* = ±0.15 has been chosen for single determinations. It should be noted that this rate constant refers to room temperature, which we estimate as T = 294 K.

**References**

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

Snook, M. E. and Hamilton, G. A.: J. Am. Chem. Soc., 96(3), 860-869, 1974.