IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_13

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

HO (aq) + (CH3)3CCH2OH (aq) → products

**Rate coefficient data**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| k/ l mol-1 s-1 | T/K | pH | | I/ mol l-1 | Reference | | | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | | | |
| 4.9 × 109 | 294 | < 2 | - | | | Walling, 1975 | Fenton reaction (a) | |

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

**Comments**

1. Radicals generated by Fenton reaction with no information on analysis; the value for the rate constant is given in table 2 as *k*3/*k*2= 12.0 with *k*3(HO + 2,2-dimethyl-1-propanol) and *k*2([HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + Fe2+) (*k*2 = 3 × 108 M-1s-1); with no exact temperature given, a room temperature of 294 K is estimated.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* /L mol-1 s-1 | 4.9 × 109 | 294 |
|  |  |  |

*Reliability*

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

*Comments on Preferred Values*

To this point, the determination by Walling (1975) is the only available for the reaction of 2,2-dimethyl-propan-1-ol with HO. In 1988, Buxton et al. recommended a rate coefficient of 4.0 × 109 M-1s-1, based on this value. While the recalculation of the original data suggests a slightly higher value, considering the estimated uncertainty of Δ log *k* = ±0.15 of ±33%, both values still agree within error limits. It has to mentioned, that Walling did not specify their methods in detail. For the estimated room temperature of 294 K it is therefore advised to follow the reevaluated determination of Walling (1975).

**References**

Buxton, G. V., Greenstock, C. L., Helman, W. P., and Ross, A. B.: J. Phys. Chem. Ref. Data, 17(2), 513-886, 1988.

Walling, C.: Acc. Chem. Res., 8(4), 125-131, 1975.