IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_13

This datasheet last evaluated: May 2017; last change in preferred values: January 2016

$OH(aq) + (CH_3)_3CCH_2OH\ (aq) \rightarrow$ products

$\Delta G_R°$ (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data $H_R°$ (g) are not available.

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	*Reference*	Technique/ Comments
Relative Rate Coefficients					
3.4×10^9		< 2		Walling, 1975	Fenton reaction (a)
4.0×10^9	298	< 2		Buxton et al., 1988	Recommended value (b)

Comments

(a) Radicals generated by Fenton reaction; no information on analysis; no information on competing reagent; the value for the rate constant is given in table 2 as $k_3/k_2 = 12.0$ with k_3(·OH + 2,2-dimethyl-1-propanol) and k_2(·OH + Fe^{2+}) ($k_2 = 3 \times 10^8$ M^{-1}s^{-1}). NIST lists this value as 5.2×10^9 M^{-1}s^{-1}, referring to k(·OH + Fe^{2+}) = 4.3×10^8 M^{-1}s^{-1}. http://kinetics.nist.gov/solution/Detail?id=1975WAL125-131:1

(b) Buxton et al. recalculated the value given by Walling (1975) as 4.0×10^9; for the Fenton reaction reference, no selected rate constant is listed.

Preferred Values

Parameter	Value	T/K
k /L mol^{-1} s^{-1}	4.0×10^9	298
Reliability		
$\Delta \log k$	± 0.04	298

Comments on Preferred Values

The former value recommended by Buxton et al. (1988) is also recommended. There have been no newer determinations. The relative error of the rate constant is estimated as ± 10 %.

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.