IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_11

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

$OH(aq) + CH_3CH_2C(CH_3)_2OH\ (aq) \rightarrow$ 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					
1.1×10^9		9		Anbar et al., 1966	CW-radiolysis /UV-vis (a)
1.9×10^9	298	9		Buxton et al., 1988	Recalculated value (b)

Comments

(a) Radicals generated by cw-irradiation, products analysed by UV-vis-spectroscopy; Reference reaction: ·OH + PNDA (p-nitrosodimethylaniline); no values given for initial concentrations; no values given for the reference rate constants; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than ±10%. NIST lists this value as 1.9×10^9 M^{-1}s^{-1}, referring to k(·OH + EtOH) = 1.9×10^9.
http://kinetics.nist.gov/solution/Detail?id=1966ANB/MEY742-747:1

(b) Buxton et al. recalculated the value determined by Anbar et al. (1966), using their selected rate constant for the reference reaction k(·OH + EtOH) = 1.9×10^9.

Preferred Values

Parameter	Value	*T*/K
k /L mol^{-1} s^{-1}	1.9×10^9	298
Reliability		
$\Delta \log k$	± 0.05	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

Anbar, M., Meyerstein, D. and Neta, P.: J. Chem. Soc. B, 742-747, 1966.

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