IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_11

The citation for this datasheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.
This datasheet last evaluated: June 2019; last change in preferred values: March 2019

HO (aq) + $CH_3CH_2C(CH_3)_2OH$ (aq) → products

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
1.9×10^9	294	9	-	Anbar et al., 1966	CW-radiolysis /UV-vis (a)

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

Comments

(a) Reference reaction: HO + PNDA (p-nitrosodimethylaniline); the reference rate constant was determined versus ethanol with k(HO + ethanol) = 1.88×10^9 $M^{-1}s^{-1}$; no values given for initial concentrations; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than ±10%; 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}	1.9×10^9	294
Reliability		
$\Delta \log k$	± 0.15	294

Comments on Preferred Values

The former value recommended by Buxton et al. (1988) is also recommended. There have been no more recent determinations. The relative error of the rate constant is estimated as ±33% or $\Delta \log k = \pm 0.15$. It should be noted that this rate constant refers to room temperature, which we estimate as T = 294 K.

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.