IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_10

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

$OH(aq) + C_2H_5CH(OH)C_2H_5\ (aq) \rightarrow$ 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					
Only relative rate coefficient	-	1.7 - 1.8	-	Snooke and Hamilton, 1974	Fenton reaction/GC-FID (a)
2.1×10^9	298	1.7 – 1.8	-	Buxton et al., 1988	Recalculated value (b)

Comments

(a) Radicals generated by Fenton reaction (I) and $S_2O_8^{2-}$ - system (II), analysed by GC-FID; cyclopentanol was used as a competing reagent; rate coefficient given as k(·OH + 3-Pentanol)/k(·OH + 2-Propanol) = 1.1 and 1.3, respectively under conditions (I) and (II) with k(·OH + 2-Propanol) = 1.0; c($FeSO_4$) = 3×10^{-3} mol/L, c($K_2S_2O_8$) = 3×10^{-3} mol/L, c(3-pentanol) given as ≥0.02 M; the ion strength cannot be determined due to the unknown acid concentration. NIST lists this value as 2.1×10^9 $M^{-1}s^{-1}$, referring to k(·OH + 2-Propanol) = 1.9×10^9 $M^{-1}s^{-1}$.
http://kinetics.nist.gov/solution/Detail?id=1974SNO/HAM860-869:24

(b) Buxton et al. used the relative value determined by Snook and Hamilton (1974) for recalculation relative to the selected rate constant for the reference reaction k(·OH + 2-propanol) = 1.9×10^9 $M^{-1}s^{-1}$.

Preferred Values

Parameter	Value	T/K
k /L mol^{-1} s^{-1}	2.1×10^9	298
Reliability		
$\Delta \log k$	± 0.04	298

Comments on Preferred Values

The recommendation of Buxton et al. (1988) is followed. The error of the room temperature 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, 12(2), 513 – 886, 1988.

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