IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_45

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

HO(aq) + $CH_3CH_2CHOHCH_2OH$(aq) → products

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
$(2.2 \pm 0.4) \times 10^9$	298	7	-	Hoffmann et al., 2009	LFP-LPA (a)
2.36×10^{11} exp[-(1400 ± 250)/T]	288 - 328	7	-		LFP-LPA (a1)

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

Comments

(a) Radicals generated by laser flash photolysis (LFP) of H_2O_2 ($c(H_2O_2) = 1 \times 10^{-4}$ M) at 248 nm; rate constant was determined to be $k = 2.3 \times 10^9$ $M^{-1}s^{-1}$, referring to reference reaction: HO + SCN^- with $k(HO + SCN^-) = 1.24 \times 10^{10}$ M^{-1} s^{-1}; the selected temperature dependence by Zhu et al. (2003) was used for recalculation; c(KSCN) = 1.59×10^{-5} M. Arrhenius expression (a1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	2.2×10^9	298
k / L mol^{-1} s^{-1}	2.36×10^{11} exp[-(1400)/T]	288 – 328

Reliability

Δ log k	±0.15	298
Δ E_A/R	±250	288 – 328

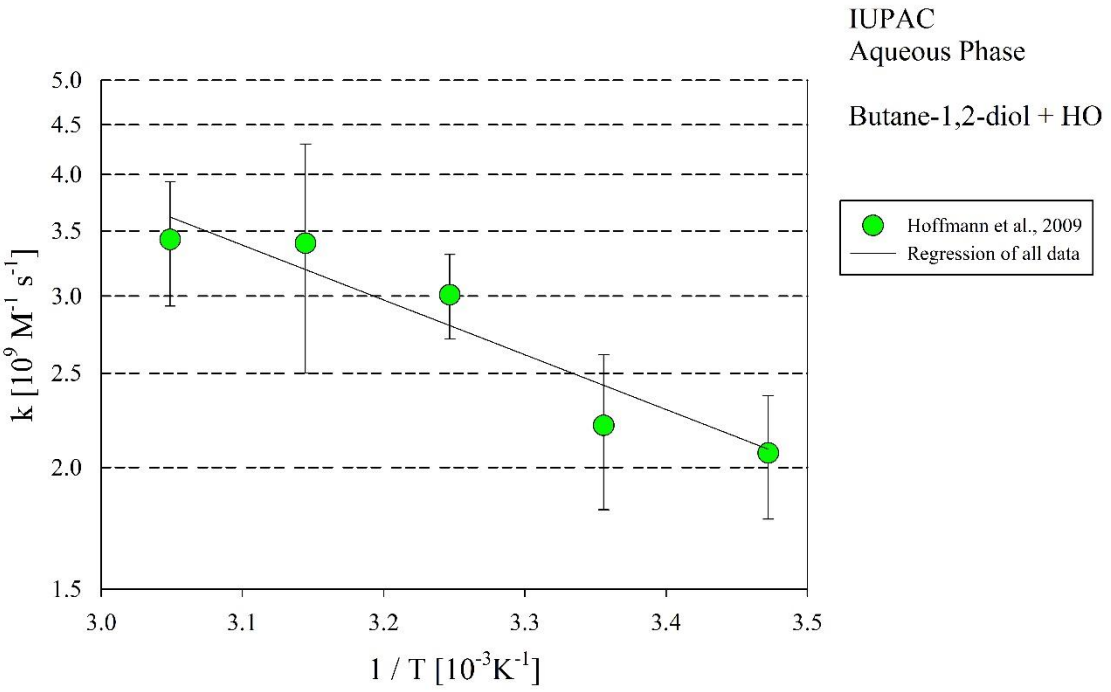
Comments on Preferred Values

The rate constants determined by Hoffmann et al. (2009) are the only ones available for the reaction of butan-1,2-diol. They have been recalculated using the recommended rate constants for the reference reaction (Zhu et al., 2003). The uncertainty is estimated to be ±20 % or Δ log k = ±0.15.

References

Hoffmann, D., Weigert, B., Barzaghi, P. and Herrmann, H.: Phys. Chem. Chem. Phys., 11, 9351-9363, 2009.

Zhu, L., Nicovich, J. M. and Wine, P. H.: Aquat. Sci., 65(4), 425-435, 2003.



T-dependent rate constants for the reaction of butane-1,2-diol with HO in aqueous solution. Data from Hoffmann et al. (2009).