

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_44

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HO(aq) + CH₃CHOH(CH₂)₂OH(aq) → products

ΔG_R° (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data H_R° (g) are not available.

Rate coefficient data

$k / \text{L mol}^{-1} \text{s}^{-1}$	T/K	pH	I/ mol L ⁻¹	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
2.17×10^9	294	-	-	Adams et al., 1965	PR / UV-Vis (a)

Comments

- (a) Referring to the reference reaction HO + SCN⁻ with $k(\text{HO} + \text{SCN}^-) = 6.6 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$; The rate constant was recalculated with the newly recommended reference rate constant $k = 1.10 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ after Zhu et al.. No exact value is given for the initial concentrations of the reactants; pH is given as natural; as no temperature is given in their publication, for room temperature of T = 294 K is assumed.

Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	2.17×10^9	294
<i>Reliability</i> $\Delta \log k$	± 0.15	294

Comments on Preferred Values

The only available room temperature rate constant determined by Adams et al. (1965) has been recalculated with the newly recommended reference rate constant, its uncertainty is estimated to be $\pm 33\%$ or $\Delta \log k = 0.15$. It should be noted that this rate coefficient refers to room temperature, which we estimate as T = 294 K.

References

Adams, G.E.; Boag, J.W.; Curren, J. and Michael, B.D., Pulse Radiolysis, Ebert, M.; Keene, J.P.; Swallow, A.J. and Baxendale, J.H. (eds.): Academic Press, New York, p.131-143, 1965.

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