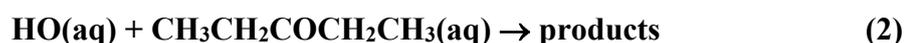


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_83

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



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>					
1.35×10^9	294	6 – 7	-	Adams et al., 1965	PR / UV-Vis (a)

The equilibrium constant for the hydration (1) has been estimated to be $K_{298 \text{ K}} = 3.8 \times 10^{-3}$ by Raventos-Duran et al. (2010).

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

Comments

- (a) Reference reaction: $\text{HO} + \text{SCN}^-$ with $k(\text{HO} + \text{SCN}^-) = 6.6 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$; for the recalculation of the rate coefficient, the selected value for the reference reaction $k = 1.10 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ was used; No exact value is given for the initial concentrations of the reactants; as no exact temperature is given, $T = 294 \text{ K}$ is assumed for room temperature.

Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	1.35×10^9	294
<i>Reliability</i>		
$\Delta \log k$	± 0.15	294

Comments on Preferred Values

The only determined rate constant for the oxidation of 3-pentanone is the one by Adams et al. (1965). This rate constant has been recalculated, using the newly recommended reference rate constant. The uncertainty of the recommendation is estimated as $\pm 33\%$ or $\Delta \log k = \pm 0.15$. It should be noted that this rate coefficient refers to room temperature, which we estimate as $T = 294 \text{ K}$.

References

Adams, G.E.; Boag, J.W.; Curren, J.; Michael, B.D., Pulse Radiolysis, Ebert, M.; Keene, J.P.; Swallow, A.J.; Baxendale, J.H. (eds.): Academic Press, New York, p.131-43, 1965.

Raventos-Duran, T., Camredon, M., Valorso, R., Mouchel-Vallon, C. and Aumont, B.: Atmos. Chem. Phys., 10(16), 7643-7654, 2010.