IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_82

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$$H_2O + CH_3(CH_2)_2COCH_3(aq) \rightarrow CH_3(CH_2)_2C(OH)_2CH_3(aq) \quad (1)$$

$$HO(aq) + CH_3(CH_2)_2COCH_3(aq) \rightarrow \text{products} \quad (2)$$

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
1.92×10^9	294	6 – 7	-	Adams et al., 1965	PR/ UV-Vis (a)

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

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

Comments

(a) Reference reaction: HO + SCN$^-$ with k(HO + SCN$^-$) = 6.6×10^9 M^{-1}s^{-1}; for the recalculation of the rate coefficient, the selected value for the reference reaction $k = 1.10 \times 10^{10}$ M^{-1}s^{-1} was used; No exact value is given for the initial concentrations of the reactants; 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}	1.92×10^9	294
Reliability		
$\Delta \log k$	±0.15	294

Comments on Preferred Values

The only determined rate constant for the aqueous phase oxidation of 2-pentanone by HO is the one of Adams et al. (1965). This rate constant has been recalculated, using the newly recommended rate constant for the reference reaction. The uncertainty of the recommended

value is estimated as ±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 K.

References

Adams, G.E.; Boag, J.W.; Currant, 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.

Buxton, G. V., Greenstock, C. L., Helman, W. P., Ross, A. B.: J. Phys. Chem. Ref. Data, Vol. 12 (2), 513 – 886, 1988.

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