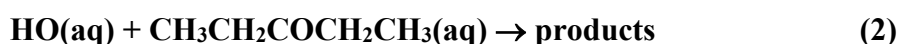


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – 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 <sup>-1</sup>	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
$1.35 \times 10^9$	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).

$\Delta G_R^\circ$  (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data  $H_R^\circ$  (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
$k / \text{L mol}^{-1} \text{s}^{-1}$	$1.35 \times 10^9$	294
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.15$	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.