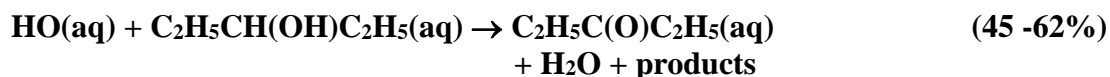


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_10

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



(Product distribution given by Snooke and Hamilton, 1974)

Rate coefficient data

$k / \text{l mol}^{-1} \text{s}^{-1}$	T/K	pH	$I / \text{mol l}^{-1}$	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
1.9×10^9	294	1.7 - 1.8	-	Snooke and Hamilton, 1974	Fenton reaction/GC- FID (a)

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

Comments

- (a) Cycloheptanol was used as a competing reagent; rate coefficient given as $k(\text{HO} + 3\text{-Pentanol})/k(\text{HO} + 2\text{-Propanol}) = 1.1$; $k(\text{HO} + 2\text{-Propanol})$ has been used as $k = 1.1 - 1.7 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$, for the re-calculation here, $k = (2.11 \times 10^9 \text{ M}^{-1}\text{s}^{-1})$ has been used as the recommended reference reaction rate constant; $c(\text{FeSO}_4) = 3 \times 10^{-3} \text{ mol/L}$, $c(\text{K}_2\text{S}_2\text{O}_8) = 3 \times 10^{-3} \text{ mol/L}$, $c(3\text{-pentanol})$ given as $\geq 0.02 \text{ M}$; as no exact temperature is given, $T = 294 \text{ K}$ is assumed for room temperature.

Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	1.9×10^9	294
<i>Reliability</i> $\Delta \log k$	± 0.15	294

Comments on Preferred Values

The only available determination by Snooke and Hamilton (1974) has been re-calculated with the recommended rate coefficient for the reference reaction. The change of the reference rate constants leads to a rate constant slightly smaller than the former recommendation by Buxton et al. (1988). The estimated uncertainty of $\pm 33\%$ or $\Delta \log k = \pm 0.15$ has been chosen for single determinations. It should be noted that this rate constant refers to room temperature, which we estimate as $T = 294 \text{ K}$.

References

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

Snook, M. E. and Hamilton, G. A.: J. Am. Chem. Soc., 96(3), 860-869, 1974.