IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_13

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

HO (aq) + $(CH_3)_3CCH_2OH$ (aq) → products

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
4.9×10^9	294	< 2	-	Walling, 1975	Fenton reaction (a)

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

Comments

(a) Radicals generated by Fenton reaction with no information on analysis; the value for the rate constant is given in table 2 as $k_3/k_2 = 12.0$ with k_3(HO + 2,2-dimethyl-1-propanol) and k_2(HO + Fe^{2+}) ($k_2 = 3 \times 10^8$ M^{-1}s^{-1}); with no exact temperature given, a room temperature of 294 K is estimated.

Preferred Values

Parameter	Value	*T*/K
k /L mol^{-1} s^{-1}	4.9×10^9	294
Reliability		
$\Delta \log k$	± 0.15	294

Comments on Preferred Values

To this point, the determination by Walling (1975) is the only available for the reaction of 2,2-dimethyl-propan-1-ol with HO. In 1988, Buxton et al. recommended a rate coefficient of 4.0×10^9 M^{-1}s^{-1}, based on this value. While the recalculation of the original data suggests a slightly higher value, considering the estimated uncertainty of $\Delta \log k = \pm 0.15$ of ±33%, both values still agree within error limits. It has to mentioned, that Walling did not specify their methods in detail. For the estimated room temperature of 294 K it is therefore advised to follow the reevaluated determination of Walling (1975).

References

Buxton, G. V., Greenstock, C. L., Helman, W. P., and Ross, A. B.: J. Phys. Chem. Ref. Data, 17(2), 513-886, 1988.

Walling, C.: Acc. Chem. Res., 8(4), 125-131, 1975.