IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_MGLY_4

This datasheet last evaluated: June 2017; last change in preferred values: March 2017

$CH_3C(O)C(OH)_2$ (aq) + CH_3NH_2 (aq)→ products

Thermochemical data not available.

Rate coefficient data ($k = k_1$)

k/ l mol^{-1} s^{-1}	T/K	*pH*	*I*/	*Reference*	Technique/ Comments
Absolute Rate Coefficients					
1.9×10^{-4}	294	3.31	0	Sedehi et al., 2013	NMR (a)
1.2×10^{-2}	298	3.84	0	Sedehi et al., 2013	NMR (a)
4.4×10^{-2}	294	5.58	0	Sedehi et al., 2013	NMR (a)

Comments

(a) The rate of this reaction was measured directly using NMR. Imidazole products were reported. The rate constants reported here were derived based on the disappearance of methylglyoxal (except for the point taken at 3.31, which is based on the appearance of imidazole). The reaction mixture initially consisted of 0.5 M methylglyoxal and 0.5 M methylamine in D_2O. pH was monitored during the reaction and average pH is reported.

Preferred Values

Parameter	Value	T/K
k / l mol^{-1} s^{-1}	10^(0.86×pH – 6.0)	294-298

Reliability

$\Delta \log k$ ± 0.3

Comments on Preferred Values

Preferred value is based on the data of Sedehi et al. (2013) as summarized in the table above. The recommendation is based on our own curve fit to the data. Parameterization is valid for $3.31 \leq pH \leq 5.58$.

References

Sedehi, N., Takano, H., Blasic, V. A., Sullivan, K. A., and De Haan, D. O.: Atmos. Environ., 77, 656, 2013.