

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_TH1\_MGLY\_3

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



Thermochemical data not available.

#### Rate coefficient data ( $k = k_1$ )

$k / 1 \text{ mol}^{-1} \text{ s}^{-1}$	$T/\text{K}$	$p\text{H}$	$I/$	<i>Reference</i>	Technique/ Comments
<i>Absolute Rate Coefficients</i>					
$2.9 \times 10^{-3}$	298	3.30	0	Sedehi et al., 2013	NMR (a)
$5.0 \times 10^{-4}$	277	3.53	0	Sedehi et al., 2013	NMR (a)
$6.3 \times 10^{-4}$	294	3.73	0	Sedehi et al., 2013	NMR (a)
$2.1 \times 10^{-2}$	298	6.54	0	Sedehi et al., 2013	NMR (a)

#### Comments

- (a) The rate of this reaction was measured directly using NMR. The rate constants reported here were derived based on the disappearance of methylglyoxal. The reaction mixture initially consisted of 0.50 M methylglyoxal and 0.50 M glycine in D<sub>2</sub>O. pH was monitored during the reaction and average pH is reported. Imidazole products were reported.

#### Preferred Values

Parameter	Value	$T/\text{K}$
$k / 1 \text{ mol}^{-1} \text{ s}^{-1}$	$1.3 \times 10^{-3}$	277-298

#### Reliability

$$\Delta \log k \quad \pm 0.3$$

#### Comments on Preferred Values

Preferred value is the average of the data of Sedehi et al. (2013) as summarized in the table above, excluding the point at pH = 6.54. No clear dependence on pH or temperature was apparent for the data. Recommendation is valid for  $3.30 \leq \text{pH} \leq 3.73$ .

## Reference

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