IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC37

This data sheet updated: 12th December 2007, (with no revision of the preferred values).

HO + $C_2H_5C(O)OH$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.8 \times 10^{-12} \exp[-(120 \pm 30)/T]$	298-440	Dagaut et al., 1988	FP-RF
$(1.22 \pm 0.12) \times 10^{-12}$	298		
$(1.07 \pm 0.05) \times 10^{-12}$	298-445	Singleton et al., 1989	PLP-RA
$(1.02 \pm 0.55) \times 10^{-12}$	298		

Preferred Values

$k = 1.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 290-450 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.

$\Delta(E/R) = \pm 300$ K.

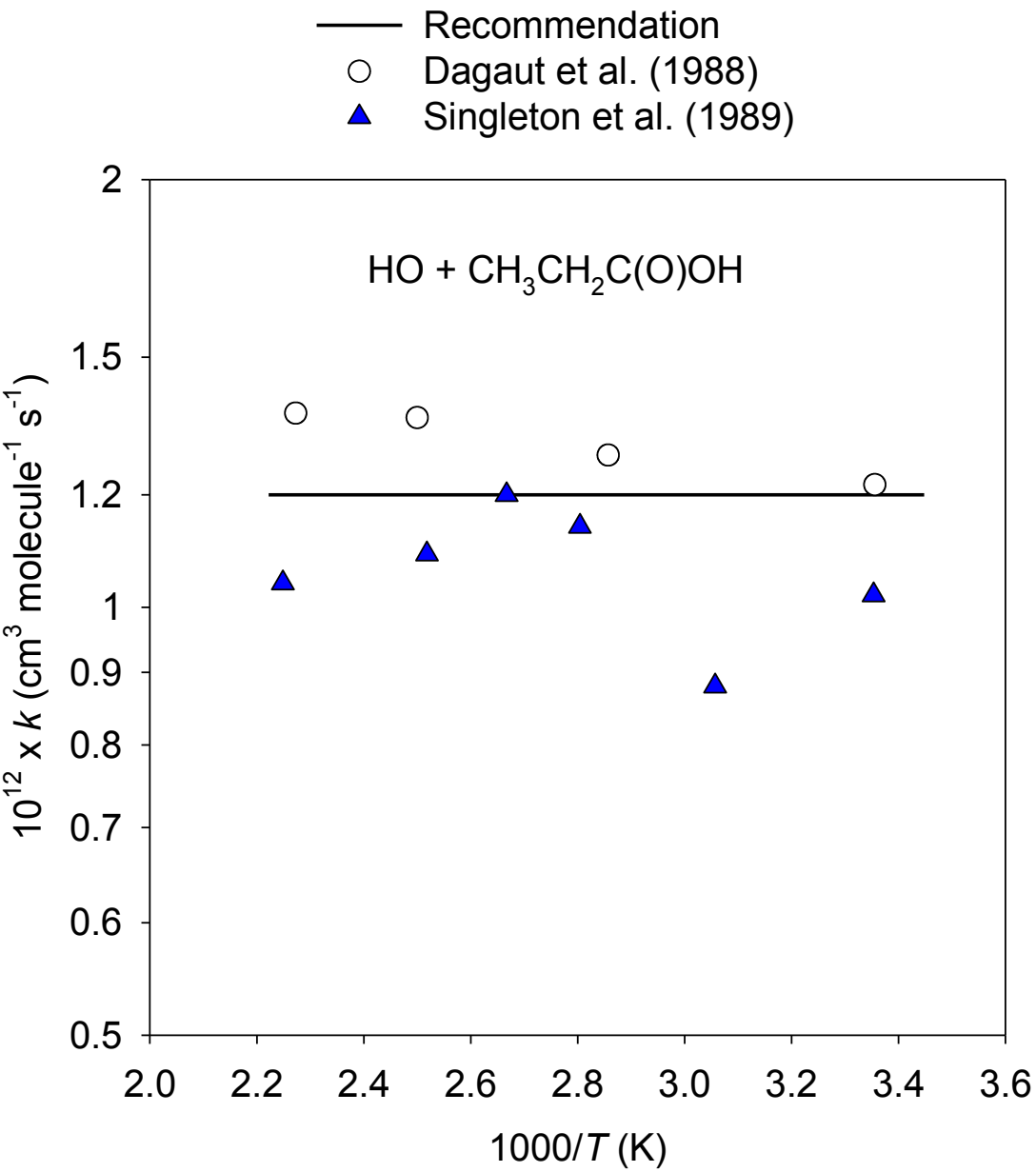
Comments on Preferred Values

The rate coefficients measured by Dagaut et al. (1988) and Singleton et al. (1989) are in good agreement and indicate that the rate coefficient for this reaction is independent of temperature over the range 298-445 K. The preferred value is an average of all of the rate coefficients of Dagaut et al. (1988) and Singleton et al. (1989), combined with a zero temperature dependence. The reaction is expected to proceed by H-atom abstraction from the C-H bonds of the $-CH_3$ group and the O-H bond of the -C(O)OH group.

References

Dagaut, P., Wallington, T. J., Liu, R. and Kurylo, M. J.: Int. J. Chem. Kinet., 20, 331, 1988.

Singleton, D. L., Paraskevopoulos, G. and Irwin, R. S.: J. Am. Chem. Soc., 111, 5248, 1989.


Recommendation
Dagaut et al. (1988)
Singleton et al. (1989)
HO + CH3CH2C(O)OH
10^12 x k (cm^3 molecule^-1 s^-1)
1000/T (K)
2
1.5
1.2
1
0.9
0.8
0.7
0.6
0.5
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6