

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.22 HI22

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### 1-C<sub>3</sub>H<sub>7</sub>OH + ice

#### Experimental data

<i>Parameter</i>	Temp./K	Reference	Technique/ Comments
<i>Partitioning coefficients: <math>K_{inc}</math></i>			
$K_{inc} = 25.6$	228	Sokolov and Abbatt, 2002	CWFT-MS (a)

#### Comments

- (a) Ice film made by freezing distilled water. Uptake was found to be reversible and equilibrium surface coverages were calculated using the geometric ice surface area. The equilibrium uptake of C<sub>3</sub>H<sub>7</sub>OH to ice at 228 K was analysed using the Langmuir isotherm. The value of  $K_{inc}$  reported in the Table was derived from values of  $K_{LangP} = 3.5 \times 10^3 \text{ Torr}^{-1}$  and  $N_{max} = 3.1 \times 10^{14} \text{ molecule cm}^{-2}$  at 228 K.

#### Preferred Values

$K_{inc} = 25.6 \text{ cm}$  at 228 K.

$N_{max} = 3.1 \times 10^{14} \text{ molecules cm}^{-2}$ , independent of temperature.

#### Reliability

$\Delta K_{inc} (228 \text{ K}) = 0.2$

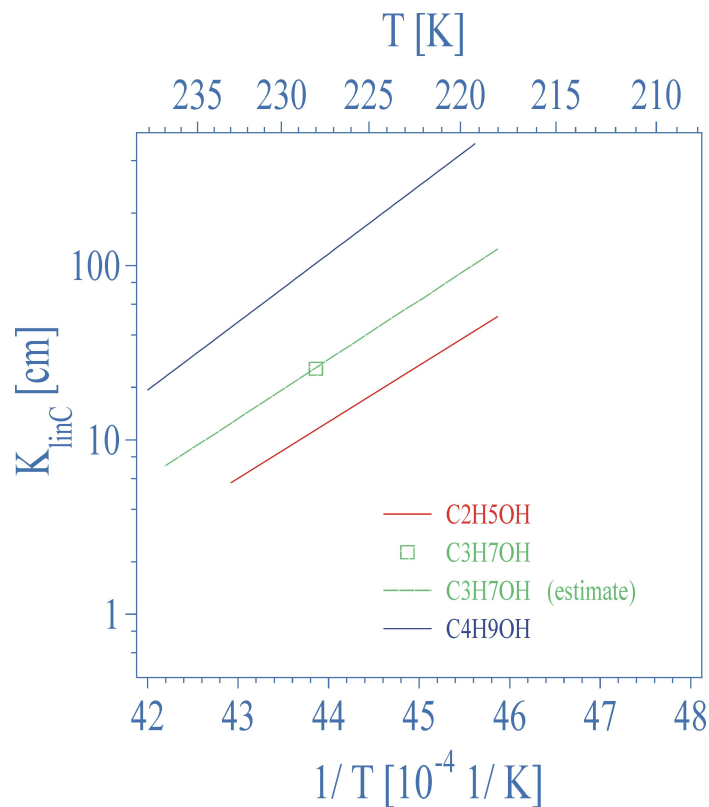
$\Delta \log N_{max} = 0.15$

#### Comments on Preferred Values

There is only one study of the reversible uptake of C<sub>3</sub>H<sub>7</sub>OH to pure ice surfaces. The value of  $N_{max}$  derived from Langmuir analyses is consistent with other straight chain alcohols (Sokolov and Abbatt, 2002). The uncertainty on the preferred values of  $K_{inc}$  and  $N_{max}$  are increased to reflect that this is the sole study to date. A rough guide to the temperature dependence of  $K_{inc}$  is:  $K_{inc} = 3.6 \times 10^{-14} \exp(7800/T)$ , which was estimated from the observed, similar temperature dependencies for C<sub>2</sub>H<sub>5</sub>OH and C<sub>4</sub>H<sub>9</sub>OH (IUPAC, 2007) and the single value at 228 K given above. In the absence of validating experimental data, this expression should however be used with caution.

## References

Sokolov, O. and Abbatt, J. P. D.: J. Phys. Chem. 106, 775-782, 2002.



Experimental values of  $K_{inc}$  for interaction of  $C_3H_7OH$  with pure ice surfaces. The preferred value,  $K_{inc} =$  at 228 K is a real measurement, the solid line assumes the temperature dependence to be similar to that observed for  $C_2H_5OH$  and  $C_4H_9OH$