

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

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1-C₃H₇OH + ice

Experimental data

<i>Parameter</i>	Temp./K	Reference	Technique/ Comments
<i>Partitioning coefficients: K_{inc}</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 C₃H₇OH 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

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

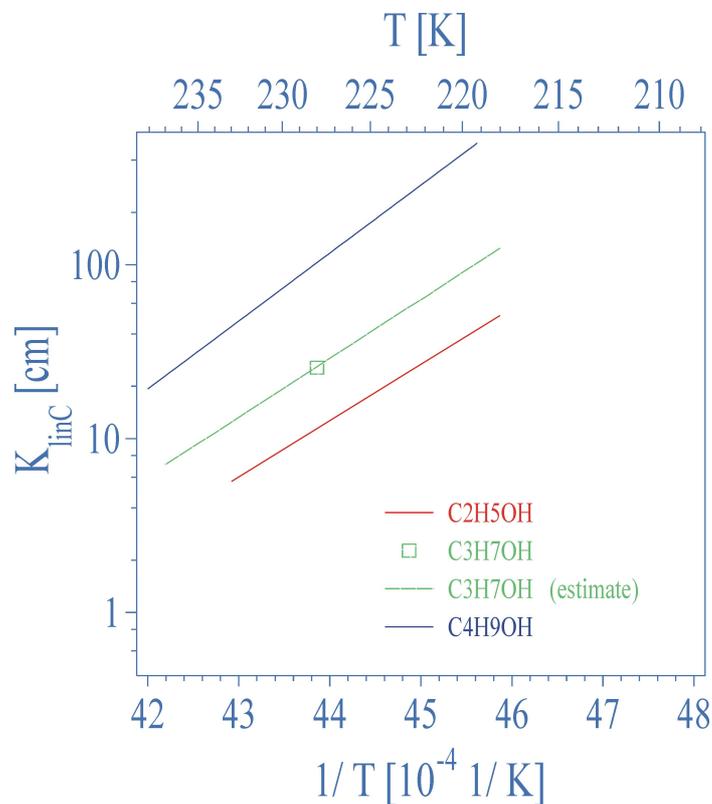
$\Delta \log N_{max} = 0.15$

Comments on Preferred Values

There is only one study of the reversible uptake of C₃H₇OH 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 C₂H₅OH and C₄H₉OH (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