Atmos. Chem. Phys. Discuss., 10, C12320–C12321, 2011
www.atmos-chem-phys-discuss.net/10/C12320/2011/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Solid state and sub-cooled liquid vapour pressures of cyclic aliphatic dicarboxylic acids" *by* A. M. Booth et al.

A. M. Booth et al.

alastair.booth@manchester.ac.uk

Received and published: 13 January 2011

We wish to thank Xinlei Ge for their helpful comment.

It seems that in this case the ACD values are not significantly better than the ones already used, except for a few cases. There is also a further, possibly more important point that as a proprietary piece of software the ACD method is something of a black box. While we can still use and evaluate it, it is very difficult to know what further measurements should be done to improve it, i.e. with the Nannoolal method we know which group-group interactions are under represented in the training set.

We have added a comment referening to the ACD method in the discussion of boiling points "Other boiling point methods are available (ACD\labs) and have been shown to

work well for certain classes of compounds, notably amines (Ge et al., 2010). However for these diacids, the ACD/labs Tb does not show a significant overall improvement compared to the Nannoolal et al., (2004) or Stein and Brown (1994) Tb (Ge, 2010), and as the mechanics of the estimation method are not disclosed, further improvement would be difficult.".

Refs Ge, X., Wexler, A. S., and Clegg, S. L.: Atmospheric Amines –Part II. Thermodynamic properties and gas/particle partitioning, Atmos. Environ., doi:10.1016/j.atmosenv.2010.10.013

Ge, X. Atmos. Chem. Phys. Discuss., 10, C10429–C10429, 2010

ACD, 2009. Software package including boiling point predictor (ACD/Tb), pKa predictor (ACD/pKa) and Solubility predictor (ACD/Solubility) used in this work, developed by Advanced Chemistry Development, Inc., 110 Youge Street, 14th floor, Toronto, Ontario, Canada M5C 1T4. http://www.acdlabs.com/home/.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 23017, 2010.