In our recent paper on the thermodynamic properties of atmospheric amines (see reference below), part of work is about the vapor pressure estimates, we also tested methods of Moller, Nannoolal and Myrdal and Yalkowsky coupled with different boliling point estimators on 58 amines with vapor pressure ranging from 10^{-6} to 1 atm.

For the boiling point predictions, we found that the ACD estimator provided the best T_b; for the vapor pressure estimates, it is hard to judge which one is better between Moller and Nannoolal methods.

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

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/.

I thought it might be valuable, if we can compare the Tb values from ACD, and see what vapor pressures can be estimated. Thus, here I provided the ACD T_b values(they also provide an error for each estimated T_b, but not sure how this error is obtained) for the compounds in this work, and used these values to predict the vapor pressures by Moller, Nannoolal and Myrdal and Yalkowsky methods, respectively.

You can find the T_b and corresponding vapor pressure estimates below, it appears that the ACD Tb values for some compunds (such as dicarboxylic acids) are much higher than both Nannoolal and Stein& brown, thus brings about large degree of underestimates of the vapor pressure.

Overall, the Moller/ACD estimates are not better than Moller/Nannoolal method—ACD T_b estimators are not very good for those compounds.

However, for some specific compound, such as **1,3-Cyclohexanedicarboxylic acid,** Cis-pinonic acid, Levoglucosan, Moller/ACD yields better results; for some compounds, such as adipic acid, suberic acid, the estimates are comparable.

It is also worthy to note that, using ACD Tb values, sometimes Nannoolal/ACD estimates are better.

I hope those additional calculations might be useful to this work.

Estimation of the boiling points

Name	ACD	Error	Nannoolal	Stein& Brown
1,1-Cyclopropanedicarboxylic acid	644.5	25	558.4	563.6
1,1-Cyclobutanedicarboxylic acid	639.6	25	573.2	579.7
1,2-cyclopentane diacarboyxlic acid	651.7	35	595.5	597.9
1,3-Cyclohexanedicarboxylic acid	605.5	25	609.6	611.6
Cis-pinonic acid	578.4	15	562.9	569.0
Levoglucosan	656.9	42	563.5	586.9
glutaric acid	576	15	573.8	569
adipic acid	611.7	15	587.9	583.5
pimelic acid	626.9	25	601.5	597
suberic acid	634.4	25	614.6	609.7
Azleaic acid	643.7	25	627.4	621.6
2-methyl succinic acid	509.7	13	563.6	559.8
2-methyl glutaric acid	605.9	0	578.1	574.8
3-methyl glutaric acid	572.1	13	578.1	574.8

Estimation of the vapor pressure using ACD predicted boiling point

Name	KEMS	Moller /ACD	Nannoolal /ACD	Myrdal and Yalkowsky /ACD
1,1-Cyclopropanedicarboxylic acid	3.10E-03	2.52E-06	1.31E-04	8.96E-04
1,1-Cyclobutanedicarboxylic acid	6.50E-03	6.30E-06	1.38E-04	1.49E-03
1,2-cyclopentane diacarboyxlic acid	3.50E-04	2.44E-06	5.16E-05	8.54E-04
1,3-Cyclohexanedicarboxylic acid	4.60E-04	2.43E-04	9.79E-04	1.51E-02
Cis-pinonic acid	7.80E-04	2.49E-03	2.27E-02	1.01E-01
Levoglucosan	1.40E-04	1.55E-03	2.89E-06	4.74E-04
glutaric acid	2.00E-03	1.05E-03	1.11E-02	4.20E-02
adipic acid	2.10E-04	6.01E-05	6.81E-04	5.03E-03
pimelic acid	2.60E-04	1.68E-05	1.62E-04	2.00E-03
suberic acid	2.20E-05	8.49E-06	6.70E-05	1.24E-03
Azleaic acid	5.10E-05	3.22E-06	2.41E-05	6.70E-04
2-methyl succinic acid	5.60E-04	2.08E-01	8.66E-01	2.26E+00
2-methyl glutaric acid	9.60E-04	1.16E-04	1.20E-03	8.19E-03
3-methyl glutaric acid	9.20E-04	2.17E-03	1.21E-02	6.24E-02