The authors test several estimation methods for ΔH(fus) ΔS(fus) and T(fus) against a set of experimental data for dicarboxylic acids. They assess the effectiveness of the estimation methods and then create a new model for the first two of these properties.

I am unable to recommend this paper for publication in Atmospheric Chemistry and Physics for the following reasons:-

1) The experimental dataset is too limited. It consists of 24 structurally very closely related compounds from 3 sets of data, 2 of which were provided by the same group using the same methods.
2) The scope of the new correlation is very limited. It is limited to $C_3$-$C_{10}$dicarboxylic acids substituted with either saturated hydrocarbon rings, methyl groups or carbonyl and/or alcohol groups. Adding, for example, mono acids would certainly expand the applicability and allow a much wider range of input data, as would adding suitable substituted mono acids.
3) The model is purely empirical- there is little attempt to analyze the experimental data and relate the modeling work to any scientific insights about (for instance) crystal packing in the solid phase or the role of molecular symmetry in determining the entropy of the liquid phase.

This work would have been fine if it had been presented in conjunction with other results (eg. additional experimental data) or alternatively the authors could have waited until further experimental data were available and then presented a model which covered a much more structurally diverse group of dicarboxylic acids from additional groups of researchers. In its present form the paper doesn't have sufficient scientific merit to warrant publication. I do however see a lot of use for being able to estimate the necessary parameters for sub-cooled liquid corrections, as it will allow us to use certain datasets which currently only have solid data. I certainly recommend addressing the points raised here.

If the paper is to be published then the following significant points should be addressed:-

Page7537, line 25:- "the difference between solid and liquid heat capacity" – "at T(fus)" should be added. Note that at T(fus) the heat capacity if infinite so Cp (solid) and Cp(liq) at T(fus) have to be obtained by extrapolation from temperatures below and above T(fus) respectively.

Page7538, lines 16-22:- What are the authors trying to do in this section? How are the standard deviations in equations 3-5 calculated and what do they mean? Lines 21-22:- How do the authors calculate that these experimental errors correspond to an uncertainty of 0.36 in log(P(l)/P(s)). Surely this quantity depends upon the absolute values of ΔH(fus), ΔS(fus) and T(fus) as well as the error in them, so which compound was used in this example? This whole section needs to be significantly clarified.

Page7538,lines 20:- The authors bring up two new sources of data on dicarboxylic acids that are not included in Table 1, nor in assessing and improving the estimation methods. Could the authors please explain this.

Page7538 ,lines 22:- it is not clear why the authors have derived the property ω problems with the oxalic acid T(fus), which could be done in other ways (eg. Plotting out T(fus) against carbon number). Can this property help to explain the variation in T(fus) and perhaps ΔH(fus) and ΔS(fus) with molecular structure via considerations of crystal packing? In the paper as it stands there is no reason to derive ω.

Page 7539, Would it be possible to estimate the ΔH(fus)for oxalic using the solid and liquid vapour pressures of soonsin et al 2010? Although there is (a lot of) disagreement about the solid VP values, the differences between the solid and liquid VP seem more consistent between the techniques, so it might be possible to back out the properties required for the sub-cooled correction.

Page7540, Eq. 10, also Page 7541, Eq. 11-14:- This is inappropriate use of the term standard deviation. Standard deviation is the measure of the scatter around a mean value. For a correlation the equivalent statistic is the standard error of estimate (SEE)(see Kachigan 1991, chapter 4) which takes a form similar to Eq. 10 except that the summation is divided by the number of degrees of freedom (not by N-1). This raises the issue of how many degrees of freedom to use in a multiple regression. Rather than using SEE or an equivalent statistic it is more usual to quote $R^2$ (also known as coefficient of determination) and to compare values between different correlations.

$$R^2 = 1 - \Sigma(y(est)-y(exp))^2/\Sigma(y(est)-y(m))^2$$

where y(est) and y(exp) are the predicted y values (from the correlation) and experimental y values respectively and y(m) is the mean of the experimental y values. Rather than quoting the PRESS statistic a cross validation $R^2$can then be quoted (using the above formula) calculated from the leave-one-out validation for the regression model.

Page7541, Section 4:-A plot of y(est) vs. y(exp) for ΔH(fus) and ΔS(fus) by the new correlations with some discussion about the distribution of residuals (particularly any outliers) should be included.

Page 7543, Section 5:- Can the authors discuss the significance of the ω values calculated for the compounds in Table 6. What is the significance of pinic acid having the lowest value and 4-oxo-pimelic acid having the highest??

Page 7543, Section 6:- Conclusions:- Authors should make it clear what are the structural limitations of the set of compounds whose properties could be estimated from these new correlations ie:- $C_3$-$C_{10}$diacids substituted with any combination of methyls/saturated rings/alcohol/ketone groups?

Table 6, can the authors add their estimate for the sub-cooled liquid vapour pressure for these compounds, I believe the solid state data is present in the literature.

Minor errors:-
Page7536,line 21:- “Vapor pressures of polyacids have been measured since decades…” I think the authors mean “over several decades”

Page7536,line 25:- “Unfortunately, pure diacids are solid at ambient temperatures…” I strongly suspect that some will be found that are not- would suggest inserting “most” after unfortunately.

Page 7537,lines 4/5:- suggest rewording to “In such cases, the activity coefficient is also needed…”

Page7538, line 3:- It might be worth saying there are 3 common ways of getting round the lack of delCp data eg, delCp = 0, 0.5delS(fus) or delS(fus)

Page7538 line 9:- Joback tends to give bad Tb data too, and M&Y (like most methods) tends to do badly with diacid vapour pressure,

Page 7538,lines14/15:- suggest rewording to “In those cases where solid-solid transitions were present the sum over all transitions was taken.”

Page 7538, Eq 3 and 4- superscript “-1” at the end of each equation.

Page7540, line 4, should this read "..., are *not* formally delH(fus) group contribution methods," otherwise I can't really follow the sentence

Page 7543,line 1:- compare Table 5 with Table 4 (not Table 3). Also $\Delta$H(fus) units in Table 4 are KJ.mol$^{-1}$ while in Table 5 they are in J.mol$^{-1}$. Consistent use of the same units would aid comparison between tables.

Page 7543, line 4 :- to improve clarity replace “these methods” with “the Section 3 methods.”

References:

Multivariate Statistical Analysis; A Conceptual Introduction, by S K Kachigan, 2nd edition, Radius Press, New York, 1991.