Subject: mean from 'n' in pKaInWater.dwar
Posted by peter on Fri, 21 May 2021 16:44:42 GMT
View Forum Message <> Reply to Message

Please could someone help me with understanding the reference data pKaInWater.dwar provided with DataWarrior?

In the method column it sometimes has "mean from n". I'm assuming this means that the pKa is the average of n experimental values? Is this correct, and if so, is there any way of obtaining the original experimental values?

Also, in the "type" column it states whether the pKa is thermodynamic or apparent. However, it sometimes has a/apparent a1/apparent b/apparent etc., and I'm not clear what the a and b stand for. I'd guess acid and base, but this doesn't seem quite right. Also, I'm not clear what the difference between a1/apparent and a2/apparent would be; do the numbers indicate different protic sites? Or do they indicate molecules with equivalent smiles but different stereochemistry? Or is it something else?

Many Thanks,

Peter