Subject: Re: Compound properties

Posted by thomas on Fri, 23 Sep 2016 21:04:34 GMT

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you are right that DataWarrior lacks a more detailled explanation of the properties. I will try to add that soon. On the other hand the counts are rather simple and often self explanatory. Hydrogen atoms are never considered, neither implicit nor explicit ones.

Hope that this quick answer helps a little,

Thomas