Subject: Re: ChemAxon calculated properties
Posted by thomas on Sun, 05 Feb 2017 22:02:59 GMT
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your procedure seems correct. I need to verify that, but I can only try with an old version, because we didn't update since quite a while.

Can you start DataWarrior from the command line? Do you get any error message then?
Are your checkboxes for pKa and LogD in the property prediction dialog enabled?
If not, then you either have a problem with the class path or you miss the file /chemaxon/marvin/calculations/pKaPlugin.class in your capka.jar?
It is part of the ChemAxon pKa-Plugin. Can you check for that class file?

Regards, Thomas