
Subject: TFA salts

Posted by [guyklx](#) on Sun, 14 Jun 2020 02:17:49 GMT

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Hi,

When copying SMILES codes for a TFA salt from ChemDraw to DW, it appears like so:

Without the charges.

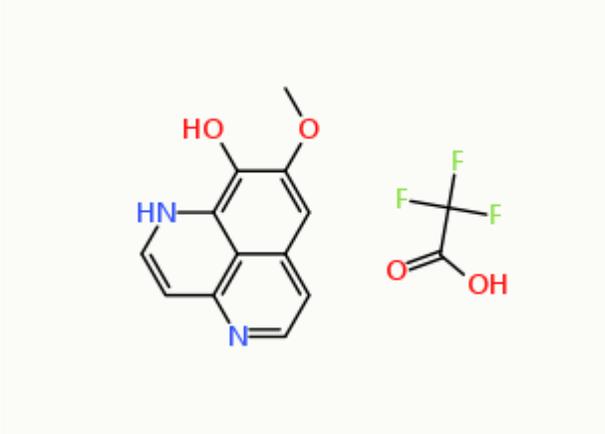
In terms of calculating chemical properties in DW (logP, PSA) for salts, should the structure be edited manually in DW to look like this?:

How exactly should I account for ion pairing in DW?

Thanks for your help,
Guy

File Attachments

1) [fromChemDraw.PNG](#), downloaded 1541 times



2) [editedDW.PNG](#), downloaded 1627 times

