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 850 times
2) editedDW.PNG, downloaded 925 times