Subject: Re: TPSA
Posted by sansun on Tue, 04 Aug 2020 10:20:26 GMT
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I performed calculations after extracting the largest fragments and used the same file for both programs.
However, I find useful information on the following link which says RDkit doesn't use P and S atoms for TPSA calculation.

Does DW uses these atoms?

https://www.rdkit.org/docs/RDKit_Book.html