Subject: Re: sp3 count
Posted by nbehrnd on Tue, 10 Aug 2021 20:24:10 GMT
View Forum Message <> Reply to Message

Dear mvamos,

based on the SMILES string generated by DW for this very structure, yet submitted to RDKit (2020.09.4) suggests different programs assign sp3-hybridization differently. In the case of RDKit, including fluorine [sic!], a total of 6.

Norwid

File Attachments

1) test_case.zip, downloaded 838 times