
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 261 times
