

Chemical blogspace is getting more chemical



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Keywords

Cb, Inchi, Pubchem

Abstract

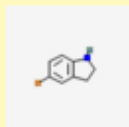
The best remedy for being depressed is the rush after hacking some nice new feature (unfortunately, it is addictive). After hacking InChI support into Chemical blogspace a couple of days back, adding some more visual feedback on those molecules is not that hard, with PubChem around that is:

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The best remedy for being depressed is the rush after hacking some nice new feature (unfortunately, it is addictive). After [hacking InChI support into Chemical blogspace](#) a couple of days back, adding some more visual feedback on [those molecules](#) is not that hard, with [PubChem](#) around that is:

5-bromo-2,3-dihydro-1H-indole



InChI: InChI=1/C8H8BrN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-2,5,10H,3-4H2
SMILES: C1CNC2=C1C=C(C=C2)Br
PubChem: [3411566](#)

Posts

Counting stereoisomers from the molecular formula



 posted to [Chem-bla-ics](#) on Sun 17th Dec 06

We all know the combinatorial explosion when calculating the number of possible cwp:structural isomorphism) of a certain molecular formula. For example, C₂H₆ has (ethane, InChI=1/C₂H₆/c1-2/h1-2H₃), and...

methane



InChI: InChI=1/CH₄/h1H₄
SMILES: C

Beware! Every [marked up molecule](#) in your blog is being picked up! So should the compound with the SMILES N(=NC1=CC=C(C=C1)N(CCO)CCO)C3=CC=C(C=CC2=C(C(=C(C#N)C#N)OC2(C)C)C#N)S3, which is [reported to be the most light sensitive molecule every synthesized so far](#).