Chemical blogspace is getting more chemical

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Citation

Keywords

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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chem-bla-ics

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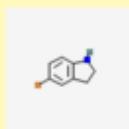
InChI: InChI=1/C8H8BrN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-2,5,10H,3-4H2
SMILES: C1CNC2=C1C=C(C=C2)Br
PubChem: 3411566

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 c wp: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 .