

chem-bla-ics

ChemSpider fail #1: SMILES

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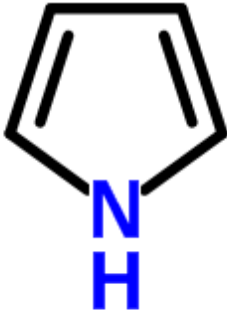
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Cheminformatics is difficult, I know. But I thought I used a simple SMILES when I typed C1CNCC1, but ChemSpider got it wrong :) The correct structure should be pyrrolidine, not pyrrole. I always mix up those names, so defaulted to ChemSpider to give me the correct name, which ChemSpider knows and where it also has the SMILES correct... there just seems something wrong with there search dialog:

Convert Load Edit

Convert from String (Name, SMILES, InChI, etc)



Ambiguous chemical name - may not correspond to the actual structure!

There has been [some talk about a ChemSpider Bugzilla](#), but I don't think this has materialized yet, and I'll have the default to info-at-chemspider-dot-com ...