

# N-Nitrosopiperidine, HFBA-derivative

**Inchi:** InChI=1S/C13H6F14N2O2/c14-8(15,10(18,19)12(22,23)24)6(30)29(28-4-2-1-3-5-28)7(31)  
**InchiKey:** MSHOFQGXEZLOC-UHFFFAOYSA-N  
**Formula:** C13H6F14N2O2  
**SMILES:** O=C(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)N1C=CCC=C1)C(F)(F)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 488.18

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.12		Crippen Method
logp	4.656		Crippen Method
mcvol	222.450	ml/mol	McGowan Method
rinpole	1410.00		NIST Webbook
rinpole	1410.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R579943&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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