

# N-Nitrosopyrrolidine, HFBA-derivative

**Inchi:** InChI=1S/C12H4F14N2O2/c13-7(14,9(17,18)11(21,22)23)5(29)28(27-3-1-2-4-27)6(30)8(31)12  
**InchiKey:** ACNNMXKAXMYNEL-UHFFFAOYSA-N  
**Formula:** C12H4F14N2O2  
**SMILES:** O=C(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)n1cccc1)C(F)(F)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 474.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	4.145		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
rinpol	1100.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R579958&Units=SI>

## Legend

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

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