

# O-Methyl-O-(1,1-difluoro-2-chloroethyl)-N-butyl-phosphorothioamide

**Inchi:** InChI=1S/C7H15ClF2NO2PS/c1-3-4-5-11-14(15,12-2)13-7(9,10)6-8/h3-6H2,1-2H3,(H,11)  
**InchiKey:** LXXYRZDQBNWFTE-UHFFFAOYSA-N  
**Formula:** C7H15ClF2NO2PS  
**SMILES:** CCCCNP(=S)(OC)OC(F)(F)CCl  
**Mol. weight [g/mol]:** 281.69

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.67		Crippen Method
logp	3.095		Crippen Method
mcvol	183.800	ml/mol	McGowan Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R544180&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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