

# O-(2-Chloro-1,1-difluoroethyl)ethanechlorothiono

**Inchi:** InChI=1S/C4H7Cl2F2OPS/c1-2-10(6,11)9-4(7,8)3-5/h2-3H2,1H3  
**InchiKey:** XLUQWXPAGAUHCX-UHFFFAOYSA-N  
**Formula:** C4H7Cl2F2OPS  
**SMILES:** CCP(=S)(Cl)OC(F)(F)CCI  
**Mol. weight [g/mol]:** 243.04

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.04		Crippen Method
logp	3.403		Crippen Method
mcvol	137.920	ml/mol	McGowan Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R544462&Units=SI>  
**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>

## 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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