

# Isothioate

**Inchi:** InChI=1S/C7H17O2PS3/c1-7(2)12-5-6-13-10(11,8-3)9-4/h7H,5-6H2,1-4H3  
**InchiKey:** SPCNPOWOBZQWJK-UHFFFAOYSA-N  
**Formula:** C7H17O2PS3  
**SMILES:** COP(=S)(OC)SCCSC(C)C  
**Mol. weight [g/mol]:** 260.38  
**CAS:** 36614-38-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.94		Crippen Method
logp	3.379		Crippen Method
mcvol	190.740	ml/mol	McGowan Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		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=C36614387&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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