

# Selenoethionine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

**Inchi:** InChI=1S/C14H27NO4Se/c1-6-18-14(17)15-12(8-9-20-7-2)13(16)19-11(5)10(3)4/h10-12  
**InchiKey:** GHDVIENQVSBWJN-JHJMLUEUSA-N  
**Formula:** C14H27NO4Se  
**SMILES:** CCOC(=O)NC(CC[Se]CC)C(=O)OC(C)C(C)C  
**Mol. weight [g/mol]:** 352.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	2.640		Crippen Method
rinpol	2039.40		NIST Webbook
rinpol	2048.80		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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R501732&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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