D-Selenomethionine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C13H25NO4Se/c1-6-17-13(16)14-11(7-8-19-5)12(15)18-10(4)9(2)3/h9-11H,6-8

InchiKey: BZJOTHGVQRKPMN-NFJWQWPMSA-N

Formula: C13H25NO4Se

SMILES: CCOC(=O)NC(CC[Se]C)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 338.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	2.249		Crippen Method
rinpol	1970.60		NIST Webbook
rinpol	1970.60		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R501950&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices