

L-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,6-8H
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 | 1980.20 | | NIST Webbook |
| rinpol | 1980.20 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R502200&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/35-260-4/L-Selenomethionine-N-O-S-ethoxycarbonyl-S-3-methyl-2-butyl-ester.pdf>

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