L-Proline, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C13H23NO4/c1-5-17-13(16)14-8-6-7-11(14)12(15)18-10(4)9(2)3/h9-11H,5-8H2

InchiKey: SYKQJQHZOPVPTP-VUWPPUDQSA-N

Formula: C13H23NO4

SMILES: CCOC(=O)N1CCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	2.195		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1697.50		NIST Webbook
rinpol	1697.50		NIST Webbook

Sources

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

Crippen Method: 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=R502191&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.