

D-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	1692.70		NIST Webbook
rinpol	1692.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R501945&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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