d-Proline, n-butoxycarbonyl-, propyl ester

Inchi: InChI=1S/C13H23NO4/c1-3-5-10-18-13(16)14-8-6-7-11(14)12(15)17-9-4-2/h11H,3-10H2
InchiKey: YADBXAIYNZVTHO-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: CCCCOC(=O)N1CCCC1C(=O)OCCC
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.341		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1741.00		NIST Webbook

Sources

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=U321079&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices