d-Proline, N-methoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C11H19NO4/c1-8(2)7-16-10(13)9-5-4-6-12(9)11(14)15-3/h8-9H,4-7H2,1-3H3
InchiKey: AJLAIKBFTCKVMT-UHFFFAOYSA-N
Formula: C11H19NO4
SMILES: COC(=O)N1CCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 229.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	1.416		Crippen Method
mcvol	179.850	ml/mol	McGowan Method
rinpol	1579.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320787&Units=SI
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

Legend

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