d-Proline, N-isobutoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C12H21NO4/c1-4-16-11(14)10-6-5-7-13(10)12(15)17-8-9(2)3/h9-10H,4-8H2,1-
InchiKey: CPUIHWCEYFMZBG-UHFFFAOYSA-N
Formula: C12H21NO4
SMILES: CCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.807		Crippen Method
mcvol	193.940	ml/mol	McGowan Method
rinpol	1620.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320801&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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