d-Proline, N-methoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C12H21NO4/c1-3-4-5-9-17-11(14)10-7-6-8-13(10)12(15)16-2/h10H,3-9H2,1-2H

InchiKey: PEJATZUDKQACFP-UHFFFAOYSA-N

Formula: C12H21NO4

SMILES: CCCCCOC(=O)C1CCCN1C(=O)OC

Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.951		Crippen Method
mcvol	193.940	ml/mol	McGowan Method
rinpol	1713.00		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=U320788&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