d-Proline, n-propoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C14H25NO4/c1-3-5-6-11-18-13(16)12-8-7-9-15(12)14(17)19-10-4-2/h12H,3-11
InchiKey: DLVJGPBUOWMEPP-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: CCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.731		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1816.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320821&Units=SI

Legend

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