d-Proline, N-allyloxycarbonyl-, butyl ester

Inchi: InChI=1S/C13H21NO4/c1-3-5-10-17-12(15)11-7-6-8-14(11)13(16)18-9-4-2/h4,11H,2-3,5-
InchiKey: GFLIZTUAONMEOE-UHFFFAOYSA-N
Formula: C13H21NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCC
Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	2.117		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320965&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.