d-Proline, N-allyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C14H23NO4/c1-3-5-6-11-18-13(16)12-8-7-9-15(12)14(17)19-10-4-2/h4,12H,2-
InchiKey: XKMQMBNOTWFWQQ-UHFFFAOYSA-N
Formula: C14H23NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCCC
Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.507		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		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=U320966&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

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