

d-Proline, N-allyloxycarbonyl-, allyl ester

Inchi: InChI=1S/C12H17NO4/c1-3-8-16-11(14)10-6-5-7-13(10)12(15)17-9-4-2/h3-4,10H,1-2,5-9
InchiKey: QYFSHFUECLCTOS-UHFFFAOYSA-N
Formula: C12H17NO4
SMILES: C=CCOC(=O)C1CCCN1C(=O)OCC=C
Mol. weight [g/mol]: 239.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	1.503		Crippen Method
mcvol	185.340	ml/mol	McGowan Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320978&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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<https://www.chemeo.com/cid/91-281-9/d-Proline-N-allyloxycarbonyl-allyl-ester.pdf>

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