

D-Proline, N-allyloxycarbonyl-, ethyl ester

Inchi: InChI=1S/C11H17NO4/c1-3-8-16-11(14)12-7-5-6-9(12)10(13)15-4-2/h3,9H,1,4-8H2,2H3
InchiKey: DJMOKWVOSMPVMX-UHFFFAOYSA-N
Formula: C11H17NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCC
Mol. weight [g/mol]: 227.26

Physical Properties

Property code	Value	Unit	Source
logp	1.337		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320963&Units=SI>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/95-175-3/D-Proline-N-allyloxycarbonyl-ethyl-ester.pdf>

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