

d-Proline, n-butoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C15H27NO4/c1-3-5-7-12-19-14(17)13-9-8-10-16(13)15(18)20-11-6-4-2/h13H,3
InchiKey: ACLZCKVVFDGTAZ-UHFFFAOYSA-N
Formula: C15H27NO4
SMILES: CCCCCOC(=O)C1CCCN1C(=O)OCCCC
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	3.121		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321082&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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