

D-Proline, N-butoxycarbonyl-, propyl ester

Inchi: InChI=1S/C13H23NO4/c1-3-5-10-18-13(16)14-8-6-7-11(14)12(15)17-9-4-2/h11H,3-10H2
InchiKey: YADBXAIYNZVTHO-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: CCCOC(=O)N1CCCC1C(=O)OCCC
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
logp	2.341		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1741.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321079&Units=SI>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/41-282-3/D-Proline-N-butoxycarbonyl-propyl-ester.pdf>

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