

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:	YADBXAIYNZVTTHO-UHFFFAOYSA-N
Formula:	C13H23NO4
SMILES:	CCCCOC(=O)N1CCCC1C(=O)OCCC
Mol. weight [g/mol]:	257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.341		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1741.00		NIST Webbook

Sources

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=U321079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/41-282-3/d-Proline-n-butoxycarbonyl-propyl-ester.pdf>

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