

d-Proline, N-methoxycarbonyl-, isobutyl ester

Inchi:	InChI=1S/C11H19NO4/c1-8(2)7-16-10(13)9-5-4-6-12(9)11(14)15-3/h8-9H,4-7H2,1-3H3
InchiKey:	AJLAIKBFTCKVMT-UHFFFAOYSA-N
Formula:	C11H19NO4
SMILES:	COC(=O)N1CCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	229.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	1.416		Crippen Method
mcvol	179.850	ml/mol	McGowan Method
rinpol	1579.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320787&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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