

Proline, N-methyl-, butyl ester

Other names:	Pro, N-methyl, butyl ester
Inchi:	InChI=1S/C10H19NO2/c1-3-4-8-13-10(12)9-6-5-7-11(9)2/h9H,3-8H2,1-2H3
InchiKey:	TXARCVDUIMCSNN-UHFFFAOYSA-N
Formula:	C10H19NO2
SMILES:	CCCCOC(=O)C1CCCN1C
Mol. weight [g/mol]:	185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	1.424		Crippen Method
mcvol	158.320	ml/mol	McGowan Method
rinpola	1328.00		NIST Webbook
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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=U152963&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/90-984-0/Proline-N-methyl-butyl-ester.pdf>

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