L-Proline, N-butyryl-, methyl ester

Inchi: InChI=1S/C10H17NO3/c1-3-5-9(12)11-7-4-6-8(11)10(13)14-2/h8H,3-7H2,1-2H3
InchiKey: YDOXTIOAUXVDHL-UHFFFAOYSA-N
Formula: C10H17NO3
SMILES: CCCC(=O)N1CCCC1C(=O)OC
Mol. weight [g/mol]: 199.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Cheméo Relay (1.0)
logp	0.951		Crippen Method
mcvol	159.890	ml/mol	McGowan Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tf	310.94	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308816&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point