Glycyl-L-Proline, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C11H19N3O3/c1-13(2)8-12-7-10(15)14-6-4-5-9(14)11(16)17-3/h8-9H,4-7H2,1-

InchiKey: ORBCDHZAMGGZQB-UHFFFAOYSA-N

Formula: C11H19N3O3

SMILES: COC(=O)C1CCCN1C(=O)CN=CN(C)C

Mol. weight [g/mol]: 241.29

Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	-0.260		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
rinpol	1994.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375723&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices