1-Methyl-4-phenyl-4-propionoxypiperidine

Other names: 3-Desmethylprodine
Inchi: InChI=1S/C15H21NO2/c1-3-14(17)18-15(9-11-16(2)12-10-15)13-7-5-4-6-8-13/h4-8H,3,9-
InchiKey: BCQMRZRAWHNSBF-UHFFFAOYSA-N
Formula: C15H21NO2
SMILES: CCC(=O)OC1(c2ccccc2)CCN(C)CC1
Mol. weight [g/mol]: 247.33
CAS: 13147-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	2.561		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	1787.00		NIST Webbook
rinpol	1787.00		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=C13147096&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

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