

1-Carbethoxy-4-phenyl-4-piperidinol

Inchi:	InChI=1S/C14H19NO2/c1-2-13(16)15-10-8-14(17,9-11-15)12-6-4-3-5-7-12/h3-7,17H,2,8
InchiKey:	GVBQDWVGDXBDTA-UHFFFAOYSA-N
Formula:	C14H19NO2
SMILES:	CCC(=O)N1CCC(O)(c2ccccc2)CC1
Mol. weight [g/mol]:	233.31
CAS:	37083-27-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	1.907		Crippen Method
mcvol	190.920	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C37083275&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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