Properidine

Other names:	4-Piperidinecarboxylic acid, 1-methyl-4-phenyl-, 1-methylethyl ester
	Isonipecotic acid, 1-methyl-4-phenyl-, isopropyl ester
	Gevelina
	Ipropethidine
	Isopedine
	Isopropyl 1-methyl-4-phenylisonipecotate
	1-Methyl-4-phenylisonipecotic acid, isopropyl ester
	1-Methyl-4-phenylpiperidine-4-carboxylic acid isopropyl ester
	Isopropyl 1-methyl-4-phenyl-4-piperidinecarboxylate
	Isopropyl 1-methyl-4-phenylpiperidine-4-carboxylate
Inchi:	InChI=1S/C16H23NO2/c1-13(2)19-15(18)16(9-11-17(3)12-10-16)14-7-5-4-6-8-14/h4-8,13
InchiKey:	XJKQCILVUHXVIQ-UHFFFAOYSA-N
Formula:	C16H23NO2
SMILES:	CC(C)OC(=O)C1(c2ccccc2)CCN(C)CC1
Mol. weight [g/mol]:	261.36
CAS:	561-76-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	2.602		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
rinpol	1750.00		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=C561762&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