Betaprodine

Other names:	4-Piperidinol, 1,3-dimethyl-4-phenyl-, propanoate (ester), trans- 4-Piperidinol, 1,3-dimethyl-4-phenyl-, propionate (ester), stereoisomer «beta»-Prodine «beta»-Prodinol Nu-1779 4-Piperidinol, 1,3-dimethyl-4-phenyl-, propanoate, trans- «beta»-1,3-Dimethyl-4-phenyl-4-propionyloxypiperidine «beta»-1,3-Dimethyl-4-phenyl-4-piperidinol propanoate 1,3-Dimethyl-4-phenyl-4-piperidinyl propionate, trans-
Inchi:	InChI=1S/C16H23NO2/c1-4-15(18)19-16(14-8-6-5-7-9-14)10-11-17(3)12-13(16)2/h5-9,13
InchiKey:	UVAZQQHAVMNMHE-BBRMVZONSA-N
Formula:	C16H23NO2
SMILES:	CCC(=O)OC1(c2ccccc2)CCN(C)CC1C
Mol. weight [g/mol]:	261.36
CAS:	468-59-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.807		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook

Sources

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=C468597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices