Trimeperidine

Other names:	Promedol
	4-Piperidinol, 1,2,5-trimethyl-4-phenyl-, propanoate (ester)
	4-Piperidinol, 1,2,5-trimethyl-4-phenyl-, propionate (ester)
	Isopromedol
	Trimeperidin
	4-Piperidinol, 1,2,5-trimethyl-4-phenyl-, propanoate
	4-Piperidinol, 1,2,5-trimethyl-4-phenyl-, propionate
	4-Piperidinol, 4-phenyl-1,2,5-trimethyl-, propionate
	1,2,5-Trimethyl-4-phenyl-4-piperidinol, propionate
	1,2,5-Trimethyl-4-phenyl-4-propionoxypiperidine
	1,2,5-Trimethyl-4-phenyl-4-propionyloxypiperidine
	Dimethylmeperidine
Inchi:	InChI=1S/C17H25NO2/c1-5-16(19)20-17(15-9-7-6-8-10-15)11-14(3)18(4)12-13(17)2/h6-
InchiKey:	UVITTYOJFDLOGI-UHFFFAOYSA-N
Formula:	C17H25NO2
SMILES:	CCC(=O)OC1(c2ccccc2)CC(C)N(C)CC1C
Mol. weight [g/mol]:	275.39
CAS:	64-39-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	3.195		Crippen Method
mcvol	233.190	ml/mol	McGowan Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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