Piperocaine

Other names:	1-Piperidinepropanol, 2-methyl-, benzoate (ester), (.+/-.)- «gamma»-(2-Methylpiperidyl)propyl benzoate (2-Methylpiperidino)propyl benzoate Metycaine Neothesin 2-Methyl-1-piperidinepropanol, benzoate 3-(2-Methyl-1-piperidyl)propyl benzoate 3-Benzoxy-1-(2-methylpiperidino)propane 1-Piperidinepropanol, 2-methyl-, benzoate, (.+/-.)- 3-(2-Methylpiperidino)propyl benzoate 1-Piperidinepropanol, 2-methyl-, benzoate (ester) Isocaine base
Inchi:	InChI=1S/C16H23NO2/c1-14-8-5-6-11-17(14)12-7-13-19-16(18)15-9-3-2-4-10-15/h2-4,9-
InchiKey:	YQKAVWCGQQXBGW-UHFFFAOYSA-N
Formula:	C16H23NO2
SMILES:	CC1CCCCN1CCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	261.36
CAS:	136-82-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	3.108		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
rinpol	1984.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1984.00		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=C136823&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