Hydroxypethidine

Other names:	4-Piperidinecarboxylic acid, 4-(3-hydroxyphenyl)-1-methyl-, ethyl ester
	Isonipecotic acid, 4-(m-hydroxyphenyl)-1-methyl-, ethyl ester
	Bemidon
	Bemidone
	Demidone
	Ethyl 4-(m-hydroxyphenyl)-1-methylisonipecotate
	Hoechst 10,446
	Hoeschst 10446
	Hydroxypethidin
	Oxipethidine
	Oxydolantin
	Oxypetidin
	Win 771
	4-Piperidinecarboxylic acid, 4-(m-hydroxyphenyl)-1-methyl-, ethyl ester
	4-(m-Hydroxyphenyl)-1-methylpiperidine-4-carboxylic acid ethyl ester
	Hoechst no. 10,446
	Biphenal
	Emidone
Inchi:	InChI=1S/C15H21NO3/c1-3-19-14(18)15(7-9-16(2)10-8-15)12-5-4-6-13(17)11-12/h4-6,11
InchiKey:	WTJBNMUWRKPFRS-UHFFFAOYSA-N
Formula:	C15H21NO3
SMILES:	CCOC(=O)C1(c2cccc(O)c2)CCN(C)CC1
Mol. weight [g/mol]:	263.33
CAS:	468-56-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.919		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		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=C468564&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