Loperamide

Other names:	Immodium
	1-Piperidinebutanamide, 4-(4-chlorophenyl)-4-hydroxy-N,N-dimethyl-«alpha»,«alpha»-diphenyl-
	4-(4-Chlorophenyl)-N,N-dimethyl-«alpha»,«alpha»-diphenyl-4-hydroxy-1-piperidinebutana
	4-(p-Chlorophenyl)-4-hydroxy-N,N-dimethyl-«alpha»,«alpha»-diphenyl-1-piperidinebutyra
Inchi:	InChI=1S/C29H33ClN2O2/c1-31(2)27(33)29(24-9-5-3-6-10-24,25-11-7-4-8-12-25)19-22-
InchiKey:	RDOIQAHITMMDAJ-UHFFFAOYSA-N
Formula:	C29H33ClN2O2
SMILES:	CN(C)C(=O)C(CCN1CCC(O)(c2ccc(Cl)cc2)CC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	477.04
CAS:	53179-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	5.088		Crippen Method
mcvol	376.970	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53179116&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from: