Lorcainide

Other names:	Benzeneacetamide, N-(4-chlorophenyl)-N-[1-(1-methylethyl)-4-piperidinyl]- 4'-Chloro-N-(1-isopropyl-4-piperidinyl)-2-phenylacetanilide
Inchi:	InChI=1S/C22H27ClN2O/c1-17(2)24-14-12-21(13-15-24)25(20-10-8-19(23)9-11-20)22(2
InchiKey:	XHOJAWVAWFHGHL-UHFFFAOYSA-N
Formula:	C22H27ClN2O
SMILES:	CC(C)N1CCC(N(C(=O)Cc2ccccc2)c2ccc(Cl)cc2)CC1
Mol. weight [g/mol]:	370.92
CAS:	59729-31-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	4.788		Crippen Method
mcvol	296.230	ml/mol	McGowan Method
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59729316&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
rinpol:	Non-polar retention indices