Levomoramide

Other names:	Pyrrolidine, 1-[3-methyl-4-(4-morpholinyl)-1-oxo-2,2-diphenylbutyl]-, (R)- Pyrrolidine, 1-(3-methyl-4-morpholino-2,2-diphenylbutyryl)-, (-)- R 898 Pyrrolidine, 1-(2,2-diphenyl-3-methyl-4-morpholinobutyryl)-, (-)- (-)-2,2-Diphenyl-3-methyl-4-morpholinobutyrylpyrrolidine Levoramide (-)-4-[2-Methyl-4-oxo-3,3-diphenyl-4-(1-pyrrolidinyl)butyl]morpholine 4-[2-Methyl-4-oxo-3,3-diphenyl-4-(1-pyrrolidinyl)butyl]morpholine, (-)- Levomoramidum
Inchi:	InChI=1S/C25H32N2O2/c1-21(20-26-16-18-29-19-17-26)25(22-10-4-2-5-11-22,23-12-6-3
InchiKey:	INUNXTSAACVKJS-NRFANRHFSA-N
Formula:	C25H32N2O2
SMILES:	CC(CN1CCOCC1)C(C(=O)N1CCCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	392.53
CAS:	5666-11-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	3.563		Crippen Method
mcvol	321.270	ml/mol	McGowan Method
rinpol	2940.00		NIST Webbook
rinpol	2980.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5666115&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