Cyclizine

Other names:	(N-Benzhydryl)(N'-methyl)diethylenediamine
	1-Diphenylmethyl-4-methylpiperazine
	1-[di(phenyl)methyl]-4-methylpiperazine
	Bw 47-83
	Ciclizina
	Compound 47-83
	Marezine
	N-Benzhydryl-N'-methylpiperazine
	N-Benzhydryl-N-methyl piperazine
	N-Methyl-N'-benzhydrylpiperazine
	N-Methyl-N'-benzyhydrylpiperazine
	NSC 26608
	Nautazine
	Ne-devomit
	Neo-devomit
	Piperazine, 1-(diphenylmethyl)-4-methyl-
	Valoid
	Wellcome preparation 47-83
	Wellcome prepn. 47-83
Inchi:	InChI=1S/C18H22N2/c1-19-12-14-20(15-13-19)18(16-8-4-2-5-9-16)17-10-6-3-7-11-17/h2
InchiKey:	UVKZSORBKUEBAZ-UHFFFAOYSA-N
Formula:	C18H22N2
SMILES:	CN1CCN(C(c2ccccc2)c2ccccc2)CC1
Mol. weight [g/mol]:	266.38
CAS:	82-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Aqueous Solubility Prediction Method
logp	3.023		Crippen Method
mcvol	226.060	ml/mol	McGowan Method
rinpol	2020.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook

rinpol	2027.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tf	378.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C82928&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

tf: Normal melting (fusion) point