Piperoxan

Other names:	1,4-Benzodioxane, 2-(piperidinomethyl)-
	Benodaine
	933F
	F933
	Fourneau 933
	Piperidine, 1-(1,4-benzodioxan-2-ylmethyl)-
	Piperidine, 1-((2,3-dihydro-1,4-benzodioxin-2-yl)methyl)-
	Piperoxane
	2-Piperidinomethyl-1,4-benzodioxane
	2-Piperidinomethyl-1,4-benzodioxan
Inchi:	InChI=1S/C14H19NO2/c1-4-8-15(9-5-1)10-12-11-16-13-6-2-3-7-14(13)17-12/h2-3,6-7,12
InchiKey:	LYKMMUBOEFYJQG-UHFFFAOYSA-N
Formula:	C14H19NO2
SMILES:	c1ccc2c(c1)OCC(CN1CCCCC1)O2
Mol. weight [g/mol]:	233.31
CAS:	59-39-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.312		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook

Sources

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=C59392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices