

1-Methyl-3-(beta-morpholinoethyl)-3-phenyloxindole

Inchi:	InChI=1S/C21H24N2O2/c1-22-19-10-6-5-9-18(19)21(20(22)24,17-7-3-2-4-8-17)11-12-23
InchiKey:	SVUKYIWICXDODR-UHFFFAOYSA-N
Formula:	C21H24N2O2
SMILES:	CN1C(=O)C(CCN2CCOCC2)(c2ccccc2)c2ccccc21
Mol. weight [g/mol]:	336.43
CAS:	94916-82-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.671		Crippen Method
mcvol	264.910	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94916822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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