MDE

Inchi: InChI=1S/C18H21NO2/c20-18(16-7-3-1-4-8-16,17-9-5-2-6-10-17)15-19-11-13-21-14-12-1
InchiKey: GJPBYSGBLBBADJ-UHFFFAOYSA-N
Formula: C18H21NO2
SMILES: OC(CN1CCOCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 283.36
CAS: 13150-37-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	2.255		Crippen Method
mcvol	227.820	ml/mol	McGowan Method
rinpol	1585.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1583.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13150373&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