Imipramine M(Dehydro-ring)

Inchi: InChI=1S/C19H22N2/c1-20(2)14-7-15-21-18-10-5-3-8-16(18)12-13-17-9-4-6-11-19(17)21
InchiKey: AFBYHZACPPSJKD-UHFFFAOYSA-N
Formula: C19H22N2
SMILES: CN(C)CCCN1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	4.260		Crippen Method
mcvol	235.850	ml/mol	McGowan Method
rinpol	1981.00		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=R213173&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