Amitriptylinoxide

Other names:	Amitriptyline N-oxide
	5H-Dibenzo(a,d)cycloheptene-«delta»5,«gamma»-propylamine, 10,11-dihydro-N,N-dimethyl-N-oxide
	Ambivalon
	Equilibrin
	1-Propanamine, 3-(10,11-dihydro-5H-dibenzo(a,d)cycloheptene-5-ylidene)-N,N-dimethyl-N-oxide
	10,11-Dihydro-N,N-dimethyl-5H-dibenzo[a,d]cycloheptene-«DELTA»5,«gamma»-propyla
	N-oxide
	3-(10,11-Dihydro-5H-dibenzo-[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine
	3-(10,11-Dihydro-5H-Dibenzo[a,d]cyclohepten-5- ylidene) -N,
	N-oxide
	N-dimethyl-1-propylamine N-oxide, 2H2O
Inchi:	InChI=1S/C20H23NO/c1-21(2,22)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(1
InchiKey:	ZPMKQFOGINQDAM-UHFFFAOYSA-N
Formula:	C20H23NO
SMILES:	C[N+](C)([O-])CCC=C1c2ccccc2CCc2ccccc21
Mol. weight [g/mol]:	293.40
CAS:	4317-14-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.181		Crippen Method
mcvol	245.830	ml/mol	McGowan Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4317140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices