DESIMIPRAMINE ACETATE

Other names:	Desipramine, N-acetyl- N-[3-(10,11-Dihydro-5H-dibenzo[b,f]azepin-5-yl)propyl]-N-methylacetamide Desipramine, acetylated
Inchi:	InChI=1S/C20H24N2O/c1-16(23)21(2)14-7-15-22-19-10-5-3-8-17(19)12-13-18-9-4-6-11-
InchiKey:	CNKJDYQMSWTPRH-UHFFFAOYSA-N
Formula:	C20H24N2O
SMILES:	CC(=O)N(C)CCCN1c2ccccc2CCc2ccccc21
Mol. weight [g/mol]:	308.42

Physical Properties

Property code	Value	Unit	Source
ie	7.37	eV	Cheméo Relay (1.0)
log10ws	-3.69		Cheméo Relay (1.0)
logp	3.792		Crippen Method
mcvol	255.810	ml/mol	McGowan Method
rinpol	2776.00		NIST Webbook
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tf	397.53	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23047269&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point