

Clomipramine

Other names:	5H-Dibenz[b,f]azepine-5-propanamine, 3-chloro-10,11-dihydro-N,N-dimethyl- 5H-Dibenz[b,f]azepine, 3-chloro-5-[3-(dimethylamino)propyl]-10,11-dihydro- Chlorimipramine G 34586 Anafranil (free base) Anafranil base Hydiphen Monochlorimipramine 3-Chloro-5-(3-(dimethylamino)propyl)-10,11-dihydro-5H-dibenz(b,f)azepine 3-Chloroimipramine 5H-Dibenz(b,f)azepine, 10,11-dihydro-3-chloro-5-(3-(dimethylamino)propyl)- NSC 169865
Inchi:	InChI=1S/C19H23ClN2/c1-21(2)12-5-13-22-18-7-4-3-6-15(18)8-9-16-10-11-17(20)14-19
InchiKey:	GDLIGKIOYRNHDA-UHFFFAOYSA-N
Formula:	C19H23ClN2
SMILES:	CN(C)CCCN1c2ccccc2CCc2ccc(Cl)cc21
Mol. weight [g/mol]:	314.85
CAS:	303-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	4.528		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2457.00		NIST Webbook
rinpol	2484.40		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2454.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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