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]: 314.86

Physical Properties

Property code	Value	Unit	Source
ie	7.43	eV	Cheméo Relay (1.0)
log10ws	-4.90		Cheméo Relay (1.0)
logp	4.528		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2405.00		NIST Webbook
rinpol	2457.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2484.40		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2454.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2457.00		NIST Webbook

rinpol	2484.40		NIST Webbook
rinpol	2454.00		NIST Webbook
tf	398.38	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C303491&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):

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