Dibenzepin

Other names:	11H-Dibenzo[b,e][1,4]diazepin-11-one, 10-[2-(dimethylamino)ethyl]-5,10-dihydro-5-methyl-
	Dibenzepine
	HF 1927
	11H-Dibenzo(b,e)(1,4)diazepin-11-one, 5,10-dihydro-10-(2-(dimethylamino)ethyl)-5-methyl-
	5H-Dibenzo(b,e)(1,4)diazepin-11(10H)-one, 10-(2-(dimethylamino)ethyl)-5-methyl-
	5,10-Dihydro-10-(2-(dimethylamino)ethyl)-5-methyl-11H-dibenzo(b,e)(1,4)diazepin-11-on
	10-(2-(Dimethylamino)ethyl)-5-methyl-5H-dibenzo(b,e)(1,4)diazepin-11(10H)-one
	10-[2-(Dimethylamino)ethyl]-5,10-dihydro-5-methyl-11-H-dibenzo[b,e][1,4]diazepin-11-on
Inchi:	InChI=1S/C18H21N3O/c1-19(2)12-13-21-17-11-7-6-10-16(17)20(3)15-9-5-4-8-14(15)18(
InchiKey:	QPGGEKPRGVJKQB-UHFFFAOYSA-N
Formula:	C18H21N3O
SMILES:	CN(C)CCN1C(=O)c2ccccc2N(C)c2ccccc21
Mol. weight [g/mol]:	295.38
CAS:	4498-32-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.976		Crippen Method
mcvol	237.610	ml/mol	McGowan Method
rinpol	2420.00		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=C4498322&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