10H-Benzo[4,5]cyclohepta[1,2-b]thiophen-10-one, 4,9-dihydro-4-(1-methyl-4-piperidinylidene)-

Other names:	Ketotifen 4,9-Dihydro-4-(1-methyl-4-piperidinylidene)-10H-benzo(4,5)cyclohepta(1,2-b)thiophen-10 HC 20-511 4,9-Dihydro-4-(1-methyl-4-piperidylidene)-10H-benzo[4,5]cyclohepta[1,2-b]thiophen-10-o
Inchi:	InChI=1S/C19H19NOS/c1-20-9-6-13(7-10-20)18-15-5-3-2-4-14(15)12-17(21)19-16(18)8-
InchiKey:	ZCVMWBYGMWKGHF-UHFFFAOYSA-N
Formula:	C19H19NOS
SMILES:	CN1CCC(=C2c3ccccc3CC(=O)c3sccc32)CC1
Mol. weight [g/mol]:	309.43
CAS:	34580-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	4.014		Crippen Method
mcvol	237.230	ml/mol	McGowan Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		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=C34580137&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

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