

Thiazesim

Other names:	1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-phenyl-5-[2-(Dimethylamino)ethyl]-2,3-dihydro-2-phenyl-1,5-benzothiazepin-4(5H)-one Tiazesim
Inchi:	InChI=1S/C19H22N2OS/c1-20(2)12-13-21-16-10-6-7-11-17(16)23-18(14-19(21)22)15-8-
InchiKey:	QJJXOEFWXSQISU-UHFFFAOYSA-N
Formula:	C19H22N2OS
SMILES:	CN(C)CCN1C(=O)CC(c2ccccc2)Sc2ccccc21
Mol. weight [g/mol]:	326.46
CAS:	5845-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.818		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5845261&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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