THIOTHIXENE

Other names:	2-(Dimethylsulfamoyl)-(9-(4-methyl-1-piperazinyl)propylidene)thioxanthene
	9H-Thioxanthene-2-sulfonamide, N,N-dimethyl-9-[3-(4-methyl-1-piperazinyl)propylidene]-
	CP 12252-1
	CP-12,252-1 base
	Cp-12,252-1
	N,N-Dimethyl-9-(3-(4-methyl-1-piperazinyl)propylidene)thiaxanthene-2-sulfonamide
	N,N-dimethyl-9-[3-(4-methylpiperazin-1-yl)propylidene]-9H-thioxanthene-2-sulphonamide
	NSC-108165
	Navan
	Navane
	Navaron
	Orbinamon
	P-4657-B
	Thiothixine
	Thioxanthene-2-sulfonamide, N,N-dimethyl-9-(3-(4-methyl-1-piperazinyl)propylidene)-
	Tiotixene
Inchi:	InChI=1S/C23H29N3O2S2/c1-24(2)30(27,28)18-10-11-23-21(17-18)19(20-7-4-5-9-22(20
InchiKey:	GFBKORZTTCHDGY-UWVJOHFNSA-N
Formula:	C23H29N3O2S2
SMILES:	CN1CCN(CC/C=C2/c3ccccc3Sc3ccc(S(=O)(=O)N(C)C)cc32)CC1
Mol. weight [g/mol]:	443.64

Physical Properties

Property code	Value	Unit	Source
ie	7.56	eV	Cheméo Relay (1.0)
log10ws	-4.24		Cheméo Relay (1.0)
logp	3.471		Crippen Method
mcvol	335.770	ml/mol	McGowan Method
tf	455.04	K	Cheméo Relay (1.0)

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5591457&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point