

Thiothixene

Other names:

9H-Thioxanthene-2-sulfonamide,
N,N-dimethyl-9-[3-(4-methyl-1-piperazinyl)propylidene]-
P-4657-B
Cp-12,252-1
CP 12252-1
CP-12,252-1 base
N,N-Dimethyl-9-(3-(4-methyl-1-piperazinyl)propylidene)thioxanthene-2-sulfonamide
Navan
Navane
Navaron
Orbinamon
Thiothixine
Thioxanthene-2-sulfonamide,
N,N-dimethyl-9-(3-(4-methyl-1-piperazinyl)propylidene)-
Thiothixene
2-(Dimethylsulfamoyl)-(9-(4-methyl-1-piperazinyl)propylidene)thioxanthene
NSC-108165
N,N-dimethyl-9-[3-(4-methylpiperazin-1-yl)propylidene]-9H-thioxanthene-2-sulphonamide

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(CCC=C2c3ccccc3Sc3ccc(S(=O)(=O)N(C)C)cc32)CC1**Mol. weight [g/mol]:** 443.62**CAS:** 5591-45-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	3.471		Crippen Method
mccvol	335.770	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5591457&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/17-411-6/Thiothixene.pdf>

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