

FLUPENTIXOL

Other names:	1-Piperazineethanol, 4-(3-(2-(trifluoromethyl)thioxanthen-9-ylidene)propyl)- 1-Piperazineethanol, 4-[3-[2-(trifluoromethyl)-9H-thioxanthen-9-ylidene]propyl]- 2-Trifluoromethyl-9-(3-(4-(«beta»-hydroxyethyl)-1-piperazinyl)propylidene)thioxanthene 2-Trifluoromethyl-9-[3-[4-(2-hydroxyethyl)piperazin-1-yl]propylidene]thioxanthene 4-(3-(2-(Trifluoromethyl)-9H-thioxanthen-9-ylidene)propyl)-1-piperazineethanol 4-(3-(2-(Trifluoromethyl)thioxanthen-9-ylidene)propyl)-1-piperazineethanol Emergil Fluanxol Flupenthixol Flupenthixole Flurentixol Fluxanxol LC 44 N 7009 Siplaril Siplarol
Inchi:	InChI=1S/C23H25F3N2OS/c24-23(25,26)17-7-8-22-20(16-17)18(19-4-1-2-6-21(19)30-22
InchiKey:	NJMYODHXAKYRHW-DVZOWYKESA-N
Formula:	C23H25F3N2OS
SMILES:	OCCN1CCN(CC/C=C2/c3ccccc3Sc3ccc(C(F)(F)F)cc32)CC1
Mol. weight [g/mol]:	434.53

Physical Properties

Property code	Value	Unit	Source
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-4.47		Cheméo Relay (1.0)
logp	4.602		Crippen Method
mcvol	308.880	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2709560&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Crippen Method:

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

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

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