ZUCLOPENTHIXOL

Other names: 1-Piperazineethanol, 4-[3-(2-chloro-9H-thioxanthen-9-ylidene)propyl]-, (Z)-
(Z)-4-[3-(2-Chlorothioxanthen-9-ylidene)propyl]-1-piperazineethanol
Inchi: InChI=1S/C22H25ClN2OS/c23-17-7-8-22-20(16-17)18(19-4-1-2-6-21(19)27-22)5-3-9-24-
InchiKey: WFPIAZLQTJBIFN-BLLMUTORSA-N
Formula: C22H25ClN2OS
SMILES: OCCN1CCN(CC/C=C2\c3ccccc3Sc3ccc(Cl)cc32)CC1
Mol. weight [g/mol]: 400.97

Physical Properties

Property code	Value	Unit	Source
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-4.50		Cheméo Relay (1.0)
logp	4.236		Crippen Method
mcvol	301.720	ml/mol	McGowan Method
tf	427.04	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53772831&Units=SI
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

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