

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:	WFPIAZLQTTJBIFN-BLLMUTORSA-N
Formula:	C22H25ClN2OS
SMILES:	OCCN1CCN(CC/C=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/ci990307I>

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

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