Thiopropazate

Other names:	1-Piperazineethanol, 4-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-, acetate (ester) 1-Piperazineethanol, 4-[3-(2-chlorophenothiazin-10-yl)propyl]-, acetate (ester) Dartal Dartalan Perphenazine acetate Thiopropazat 1-Piperazineethanol, 4-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-, acetate 1-Piperazineethanol, 4-(3-(2-chlorophenothiazin-10-yl)propyl)-, acetate 4-(3-(2-Chlorophenothiazin-10-yl)propyl)-1-piperazineethanol acetate 1-(2-Acetoxyethyl)-4-[3-(2-chloro-10-phenothiazinyl)propyl]piperazine 10-[3-[4-(2-Acetoxyethyl)-1-piperazinyl]propyl]-2-chlorophenothiazine 2-Chloro-10-[3-[1-(2-acetoxyethyl)-4-piperazinyl]propyl]phenothiazine N-(«beta»-Acetoxyethyl)-N'-(«gamma»-(2'-chloro-10'-phenothiazinyl)propyl)piperazine Perphenazine, monoacetylated
Inchi:	InChI=1S/C23H28ClN3O2S/c1-18(28)29-16-15-26-13-11-25(12-14-26)9-4-10-27-20-5-2-
InchiKey:	AIUHRQHVWSUTGJ-UHFFFAOYSA-N
Formula:	C23H28ClN3O2S
SMILES:	CC(=O)OCCN1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc32)CC1
Mol. weight [g/mol]:	446.00
CAS:	84-06-0

Physical Properties

Property code	Value	Unit	Source
ie	7.31 ± 0.14	eV	NIST Webbook
log10ws	-4.61		Crippen Method
logp	4.513		Crippen Method
mcvol	331.660	ml/mol	McGowan Method
rinpol	3480.00		NIST Webbook
rinpol	3468.00		NIST Webbook
rinpol	3468.00		NIST Webbook
rinpol	3465.00		NIST Webbook
rinpol	3465.00		NIST Webbook
rinpol	3468.00		NIST Webbook
rinpol	3480.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices