

Thiethylperazine

Other names:	10H-Phenothiazine, 2-(ethylthio)-10-[3-(4-methyl-1-piperazinyl)propyl]- Phenothiazine, 2-(ethylthio)-10-[3-(4-methyl-1-piperazinyl)propyl]- Ethylthioperazine 2-(Ethylthio)-10-[3-(4-methyl-1-piperazinyl)propyl]phenothiazine 2-(Ethylthio)-10-[3-(4-methyl-1-piperazinyl)propyl]phenthiazine
Inchi:	InChI=1S/C22H29N3S2/c1-3-26-18-9-10-22-20(17-18)25(19-7-4-5-8-21(19)27-22)12-6-1
InchiKey:	XCTYLCDETVUOIP-UHFFFAOYSA-N
Formula:	C22H29N3S2
SMILES:	CCSc1ccc2c(c1)N(CCCN1CCN(C)CC1)c1cccc1S2
Mol. weight [g/mol]:	399.62
CAS:	1420-55-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	5.039		Crippen Method
mcvol	314.240	ml/mol	McGowan Method
rinpol	3247.00		NIST Webbook
rinpol	3247.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3240.00		NIST Webbook
rinpol	3205.00		NIST Webbook
rinpol	3210.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1420559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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