BUTAPERAZINE

Other names:	1-Butanone, 1-[10-[3-(4-methyl-1-piperazinyl)propyl]-10H-phenothiazin-2-yl]- 1-Butanone, 1-(10-(3-(4-methyl-1-piperazinyl)propyl)phenothiazin-2-yl)- AHR-712 Bayer 1362 3-n-Butyryl-10-(3'-N-methyl-piperazino-N'-propyl)phenothiazine Butyrylperazine Emerex Megalectil 1-(10-(3-(4-Methyl-1-piperazinyl)propyl)phenothiazin-2-yl)-1-butanone Randolectil Repoise Riker 595 Tyrylen AHR-3000 2-Butyryl-10-[3-(4-methyl-1-piperazinyl)propyl]phenothiazine Perazine, (1-oxobutyl)-
Inchi:	InChI=1S/C24H31N3OS/c1-3-7-22(28)19-10-11-24-21(18-19)27(20-8-4-5-9-23(20)29-24
InchiKey:	DVLBYTMYSMAKHP-UHFFFAOYSA-N
Formula:	C24H31N3OS
SMILES:	CCCC(=O)c1ccc2c(c1)N(CCCN1CCN(C)CC1)c1ccccc1S2
Mol. weight [g/mol]:	409.60

Physical Properties

Property code	Value	Unit	Source
ie	7.38	eV	Cheméo Relay (1.0)
log10ws	-4.58		Cheméo Relay (1.0)
logp	4.910		Crippen Method
mcvol	327.640	ml/mol	McGowan Method
rinpol	3188.00		NIST Webbook
rinpol	3188.00		NIST Webbook
tf	395.48	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C653032&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
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point