

Butaperazine

Other names:	1-Butanone, 1-[10-[3-(4-methyl-1-piperaziny)propyl]-10H-phenothiazin-2-yl]- 1-Butanone, 1-(10-(3-(4-methyl-1-piperaziny)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-piperaziny)propyl)phenothiazin-2-yl)-1-butanone Randolectil Repoise Riker 595 Tyrylen AHR-3000 2-Butyryl-10-[3-(4-methyl-1-piperaziny)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)c1cccc1S2
Mol. weight [g/mol]:	409.59
CAS:	653-03-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	4.910		Crippen Method
mcvol	327.640	ml/mol	McGowan Method
rinpol	3188.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C653032&Units=SI>

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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