

Perazine M (HO-), monoacetylated

Inchi:	InChI=1S/C23H28N2O2S/c1-17(26)27-19-9-10-21-23(16-19)28-22-8-4-3-7-20(22)25(21)
InchiKey:	HKSUBLQLPOCWAX-UHFFFAOYSA-N
Formula:	C23H28N2O2S
SMILES:	CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CCCC1CCN(C)CC1
Mol. weight [g/mol]:	396.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	5.337		Crippen Method
mcvol	309.440	ml/mol	McGowan Method
rinpol	3190.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R310462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/34-440-5/Perazine-M-HO-monoacetylated.pdf>

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