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/ci990307l
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