Thioridazine M (nor-), monoacetylated

Inchi: InChI=1S/C22H26N2OS2/c1-16(25)23-13-6-5-7-17(23)12-14-24-19-8-3-4-9-21(19)27-22-
InchiKey: YCDMQFVMNFYJQK-UHFFFAOYSA-N
Formula: C22H26N2OS2
SMILES: CSc1ccc2c(c1)N(CCC1CCCCN1C(C)=O)c1ccccc1S2
Mol. weight [g/mol]: 398.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	5.802		Crippen Method
mcvol	305.830	ml/mol	McGowan Method
rinpol	3490.00		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=R310704&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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