Periciazine, monoacetylated

Inchi: InChI=1S/C23H25N3O2S/c1-17(27)28-19-9-13-25(14-10-19)11-4-12-26-20-5-2-3-6-22(2
InchiKey: JCSGAMXIJYDBPZ-UHFFFAOYSA-N
Formula: C23H25N3O2S
SMILES: CC(=O)OC1CCN(CCCN2c3ccccc3Sc3ccc(C#N)cc32)CC1
Mol. weight [g/mol]: 407.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	4.579		Crippen Method
mcvol	310.820	ml/mol	McGowan Method
rinpol	3391.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310482&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices