Pecazine M (nor-HO-), diacetylated

Inchi: InChI=1S/C22H24N2O3S/c1-15(25)23-11-5-6-17(13-23)14-24-19-7-3-4-8-21(19)28-22-1
InchiKey: PRKZGISUABQNLC-UHFFFAOYSA-N
Formula: C22H24N2O3S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC1CCCN(C(C)=O)C1
Mol. weight [g/mol]: 396.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.473		Crippen Method
mcvol	296.920	ml/mol	McGowan Method
rinpol	3414.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310457&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