Pecazine M (HO-), monoacetylated

Inchi: InChI=1S/C21H24N2O2S/c1-15(24)25-17-9-10-19-21(12-17)26-20-8-4-3-7-18(20)23(19)
InchiKey: CJFTUQHGQYCMGK-UHFFFAOYSA-N
Formula: C21H24N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC1CCCN(C)C1
Mol. weight [g/mol]: 368.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	4.556		Crippen Method
mcvol	281.260	ml/mol	McGowan Method
rinpol	2750.00		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=R310437&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