Dixyrazine M (N-desalkyl-), monoacetylated

Inchi: InChI=1S/C22H27N3OS/c1-17(15-23-11-13-24(14-12-23)18(2)26)16-25-19-7-3-5-9-21(19
InchiKey: IWUDTDLFXWNRAY-UHFFFAOYSA-N
Formula: C22H27N3OS
SMILES: CC(=O)N1CCN(CC(C)CN2c3ccccc3Sc3ccccc32)CC1
Mol. weight [g/mol]: 381.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	4.089		Crippen Method
mcvol	299.460	ml/mol	McGowan Method
rinpol	3355.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310284&Units=SI

Legend

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