Dixyrazine, monoacetylated

Inchi: InChI=1S/C26H35N3O3S/c1-21(19-28-13-11-27(12-14-28)15-16-31-17-18-32-22(2)30)20
InchiKey: LAHKSILSJFAQLI-UHFFFAOYSA-N
Formula: C26H35N3O3S
SMILES: CC(=O)OCCOCCN1CCN(CC(C)CN2c3ccccc3Sc3ccccc32)CC1
Mol. weight [g/mol]: 469.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	4.123		Crippen Method
mcvol	367.560	ml/mol	McGowan Method
rinpol	3531.00		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=R310308&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