Mequitazine M (hydroxy-sulfoxide), acetylated

Inchi: InChI=1S/C22H24N2O3S/c1-15(25)27-18-6-7-20-22(12-18)28(26)21-5-3-2-4-19(21)24(2
InchiKey: SLKAFYLNGOWJJB-UHFFFAOYSA-N
Formula: C22H24N2O3S
SMILES: CC(=O)Oc1ccc2c(c1)S(=O)c1ccccc1N2CC1CN2CCC1CC2
Mol. weight [g/mol]: 396.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	3.572		Crippen Method
mcvol	290.360	ml/mol	McGowan Method
rinpol	3230.00		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=R314419&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