Sulforidazine M (nor-), monoacetylated

Inchi: InChI=1S/C22H26N2O3S2/c1-16(25)23-13-6-5-7-17(23)12-14-24-19-8-3-4-9-21(19)28-2
InchiKey: VPKWFQLEEXLAAT-UHFFFAOYSA-N
Formula: C22H26N2O3S2
SMILES: CC(=O)N1CCCCC1CCN1c2ccccc2Sc2ccc(S(C)(=O)=O)cc21
Mol. weight [g/mol]: 430.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	4.484		Crippen Method
mcvol	317.570	ml/mol	McGowan Method
rinpol	3800.00		NIST Webbook
rinpol	3800.00		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=R310640&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

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