Acepromazine, (nor-), monoacetylated

Inchi: InChI=1S/C20H22N2O2S/c1-14(23)16-9-10-20-18(13-16)22(12-6-11-21(3)15(2)24)17-7-4

InchiKey: AAOIVBNHRFXGKR-UHFFFAOYSA-N

Formula: C20H22N2O2S

SMILES: CC(=O)c1ccc2c(c1)N(CCCN(C)C(C)=O)c1ccccc1S2

Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	4.360		Crippen Method
mcvol	273.730	ml/mol	McGowan Method
rinpol	3143.00		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=R310086&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