Acepromethazine M (HO-), monoacetylated

Inchi: InChI=1S/C22H26N2O3S/c1-14(12-23(4)5)13-24-19-8-7-18(27-16(3)26)11-22(19)28-21-9

InchiKey: QFDMUHWKQLFCED-UHFFFAOYSA-N

Formula: C22H26N2O3S

SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccc(C(C)=O)cc1N2CC(C)CN(C)C

Mol. weight [g/mol]: 398.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	4.615		Crippen Method
mcvol	307.780	ml/mol	McGowan Method
rinpol	3026.00		NIST Webbook
rinpol	3026.00		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=R310100&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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