Levomepromazine M (nor-), monoacetylated

Inchi: InChI=1S/C20H24N2O2S/c1-14(12-21(3)15(2)23)13-22-17-7-5-6-8-19(17)25-20-10-9-16
InchiKey: OHFIMZCYCAXBAY-AWEZNQCLSA-N
Formula: C20H24N2O2S
SMILES: COc1ccc2c(c1)N(CC(C)CN(C)C(C)=O)c1ccccc1S2
Mol. weight [g/mol]: 356.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	4.412		Crippen Method
mcvol	278.030	ml/mol	McGowan Method
rinpol	2970.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310393&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices