Acepromethazine M (nor-), monoacetylated

Inchi: InChI=1S/C21H24N2O2S/c1-14(12-22(4)16(3)25)13-23-18-7-5-6-8-20(18)26-21-10-9-17(
InchiKey: DOFVXANYKILRNP-UHFFFAOYSA-N
Formula: C21H24N2O2S
SMILES: CC(=O)c1ccc2c(c1)N(CC(C)CN(C)C(C)=O)c1ccccc1S2
Mol. weight [g/mol]: 368.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	4.606		Crippen Method
mcvol	287.820	ml/mol	McGowan Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		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=R310115&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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