Acepromazine, M (OH-), monoacetylated

Inchi: InChI=1S/C21H24N2O3S/c1-14(24)16-6-9-20-19(12-16)23(11-5-10-22(3)4)18-8-7-17(26-
InchiKey: ADKWGZFJUSHRNY-UHFFFAOYSA-N
Formula: C21H24N2O3S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccc(C(C)=O)cc1N2CCCN(C)C
Mol. weight [g/mol]: 384.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.369		Crippen Method
mcvol	293.690	ml/mol	McGowan Method
rinpol	3041.00		NIST Webbook
rinpol	3041.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310071&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.