

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-
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
rinpola	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
rinpola: Non-polar retention indices

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