Acepromazine, M(dihydro-), monoacetylated

Inchi: InChI=1S/C21H26N2O2S/c1-15(25-16(2)24)17-10-11-21-19(14-17)23(13-7-12-22(3)4)18
InchiKey: BONMTFCWSFUEJO-UHFFFAOYSA-N
Formula: C21H26N2O2S
SMILES: CC(=O)OC(C)c1ccc2c(c1)N(CCCN(C)C)c1ccccc1S2
Mol. weight [g/mol]: 370.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	4.865		Crippen Method
mcvol	292.120	ml/mol	McGowan Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310066&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

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