Oxomemazine M (nor-), acetylated

Inchi: InChI=1S/C19H22N2O3S/c1-14(12-20(3)15(2)22)13-21-16-8-4-6-10-18(16)25(23,24)19-
InchiKey: OFFLAQXVJUTPHQ-UHFFFAOYSA-N
Formula: C19H22N2O3S
SMILES: CC(=O)N(C)CC(C)CN1c2ccccc2S(=O)(=O)c2ccccc21
Mol. weight [g/mol]: 358.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	3.085		Crippen Method
mcvol	269.810	ml/mol	McGowan Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		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=R314464&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.