1-Acetyl-4-(2-acetoxyphenyl)piperazine

Other names: Piperazine, 1-(2-acetoxyphenyl)-4-acetyl
Inchi: InChI=1S/C14H18N2O3/c1-11(17)15-7-9-16(10-8-15)13-5-3-4-6-14(13)19-12(2)18/h3-6H
InchiKey: PJPNYBPVOVTOKS-UHFFFAOYSA-N
Formula: C14H18N2O3
SMILES: CC(=O)Oc1ccccc1N1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	1.280		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		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=U280840&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