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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U280840&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

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