Piperazine, 1-(1,3-benzodioxol-5-ylmethyl)-4-acetyl

Other names: 1-(3,4-methelenedioxybenzyl)piperazine, N-acetyl
Inchi: InChI=1S/C14H18N2O3/c1-11(17)16-6-4-15(5-7-16)9-12-2-3-13-14(8-12)19-10-18-13/h2
InchiKey: AQKVLYAIWJEPQY-UHFFFAOYSA-N
Formula: C14H18N2O3
SMILES: CC(=O)N1CCN(Cc2ccc3c(c2)OCO3)CC1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.079		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R408836&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