1-[3,4-methylenedioxy-benzyl]piperazine -M, (desmethylen-methyl-), 2AC

Other names: Piperazine, 1-(4-acetoxy-3-methoxyphenylmethyl)-4-acetyl
Piperazine, 1-(4-acetoxy-3-methoxybenzyl)-4-acetyl

Inchi: InChI=1S/C16H22N2O4/c1-12(19)18-8-6-17(7-9-18)11-14-4-5-15(22-13(2)20)16(10-14)2

InchiKey: QAOSQOHAMGWDFY-UHFFFAOYSA-N

Formula: C16H22N2O4

SMILES: COc1cc(CN2CCN(C(C)=O)CC2)ccc1OC(C)=O

Mol. weight [g/mol]: 306.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	1.285		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R284254&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