

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/ci9903071>

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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