1-(4-methoxyphenyl)piperazine, acetyl

Other names:	pMeOPP, AC
	Piperazine, 1-(4-methoxyphenyl), 4-acetyl
Inchi:	InChI=1S/C13H18N2O2/c1-11(16)14-7-9-15(10-8-14)12-3-5-13(17-2)6-4-12/h3-6H,7-10H
InchiKey:	AVCQLYXAEKNILW-UHFFFAOYSA-N
Formula:	C13H18N2O2
SMILES:	COc1ccc(N2CCN(C(C)=O)CC2)cc1
Mol. weight [g/mol]:	234.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	1.364		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		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=U379035&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