

Piperazine, 1-(2-methoxyphenyl)-4-acetyl

Inchi: InChI=1S/C13H18N2O2/c1-11(16)14-7-9-15(10-8-14)12-5-3-4-6-13(12)17-2/h3-6H,7-10H
InchiKey: ZKKQCNJWCNXXKGN-UHFFFAOYSA-N
Formula: C13H18N2O2
SMILES: COc1ccccc1N1CCN(C(C)=O)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	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R404443&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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<https://www.chemeo.com/cid/19-185-6/Piperazine-1-2-methoxyphenyl-4-acetyl.pdf>

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