Ethanone, 1-(4-phenyl-1-piperazinyl)-

Other names: Piperazine, 1-phenyl, 4-acetyl
Inchi: InChI=1S/C12H16N2O/c1-11(15)13-7-9-14(10-8-13)12-5-3-2-4-6-12/h2-6H,7-10H2,1H3
InchiKey: YFBOBXSXWBMZCY-UHFFFAOYSA-N
Formula: C12H16N2O
SMILES: CC(=O)N1CCN(c2ccccc2)CC1
Mol. weight [g/mol]: 204.27
CAS: 21557-13-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	1.355		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1872.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21557131&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices