Benzylpiperazine, AC

Inchi: InChI=1S/C13H18N2O/c1-12(16)15-9-7-14(8-10-15)11-13-5-3-2-4-6-13/h2-6H,7-11H2,1H
InchiKey: FNLXJRLWMCLBRC-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: CC(=O)N1CCN(Cc2ccccc2)CC1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.67		Crippen Method
logp	1.351		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		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=R284269&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

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