N-methyl-n'-phenacylpiperazine

Inchi: InChI=1S/C13H18N2O/c1-14-7-9-15(10-8-14)11-13(16)12-5-3-2-4-6-12/h2-6H,7-11H2,1H
InchiKey: LJTXXCLPBZQLHW-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: CN1CCN(CC(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 218.29
CAS: 41298-85-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.26		Crippen Method
logp	1.117		Crippen Method
mcvol	180.940	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41298855&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