5-Chloro-2-piperidyl-acetanilide

Inchi: InChI=1S/C13H17ClN2O/c1-10(17)15-12-9-11(14)5-6-13(12)16-7-3-2-4-8-16/h5-6,9H,2-4
InchiKey: MNQXXDBLEOCASW-UHFFFAOYSA-N
Formula: C13H17ClN2O
SMILES: CC(=O)Nc1cc(Cl)ccc1N1CCCCC1
Mol. weight [g/mol]: 252.74
CAS: 116495-98-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	3.289		Crippen Method
mcvol	193.180	ml/mol	McGowan Method

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=C116495988&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