Tetrahydrorhombipholine

Inchi: InChI=1S/C15H24N2O/c1-2-3-7-16-9-12-8-13(11-16)14-5-4-6-15(18)17(14)10-12/h2,12-1
InchiKey: OKTIETCHYDTVGN-AMIUJLCOSA-N
Formula: C15H24N2O
SMILES: C=CCCN1CC2CC(C1)C1CCCC(=O)N1C2
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	1.895		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
rinpol	2050.00		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=R546631&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