Piperidine, 1-heptyl-2-methyl

Inchi: InChI=1S/C13H27N/c1-3-4-5-6-8-11-14-12-9-7-10-13(14)2/h13H,3-12H2,1-2H3
InchiKey: TVWNFLSBTYOFGL-UHFFFAOYSA-N
Formula: C13H27N
SMILES: CCCCCCCN1CCCCC1C
Mol. weight [g/mol]: 197.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.831		Crippen Method
mcvol	193.150	ml/mol	McGowan Method
rinpol	1386.00		NIST Webbook
ripol	1496.00		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=R222038&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
ripol: Polar retention indices