Piperidine, 1-heptyl-2,6-dimethyl

Inchi: InChI=1S/C14H29N/c1-4-5-6-7-8-12-15-13(2)10-9-11-14(15)3/h13-14H,4-12H2,1-3H3
InchiKey: PPJIADJRZYKHPE-UHFFFAOYSA-N
Formula: C14H29N
SMILES: CCCCCCCN1C(C)CCCC1C
Mol. weight [g/mol]: 211.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	4.220		Crippen Method
mcvol	207.240	ml/mol	McGowan Method
rinpol	1456.00		NIST Webbook
ripol	1566.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R222023&Units=SI

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