Piperidine, 2,6-dimethyl-1-pentyl

Inchi: InChI=1S/C12H25N/c1-4-5-6-10-13-11(2)8-7-9-12(13)3/h11-12H,4-10H2,1-3H3
InchiKey: IKKXYXMVMBCQJF-UHFFFAOYSA-N
Formula: C12H25N
SMILES: CCCCCN1C(C)CCCC1C
Mol. weight [g/mol]: 183.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.440		Crippen Method
mcvol	179.060	ml/mol	McGowan Method
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
ripol	1373.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R222127&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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