

Piperidine, 1-butyl-2,6-dimethyl

Inchi: InChI=1S/C11H23N/c1-4-5-9-12-10(2)7-6-8-11(12)3/h10-11H,4-9H2,1-3H3
InchiKey: CZYJDLBKBPRAIJ-UHFFFAOYSA-N
Formula: C11H23N
SMILES: CCCC1C(C)CCCC1C
Mol. weight [g/mol]: 169.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	3.049		Crippen Method
mcvol	164.970	ml/mol	McGowan Method
rinpol	1166.00		NIST Webbook
rinpol	1166.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		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=R221966&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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