

Piperidine, 1-butyl-4-methyl

Inchi: InChI=1S/C10H21N/c1-3-4-7-11-8-5-10(2)6-9-11/h10H,3-9H2,1-2H3
InchiKey: AXMCYIWXDKWDCL-UHFFFAOYSA-N
Formula: C10H21N
SMILES: CCCC1CCC(C)CC1
Mol. weight [g/mol]: 155.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	2.518		Crippen Method
mcvol	150.880	ml/mol	McGowan Method
rinpol	1082.00		NIST Webbook
ripol	1190.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R221991&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

Latest version available from:

<https://www.chemeo.com/cid/78-780-0/Piperidine-1-butyl-4-methyl.pdf>

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