

Piperidine, 1-butyl-3-methyl

Inchi: InChI=1S/C10H21N/c1-3-4-7-11-8-5-6-10(2)9-11/h10H,3-9H2,1-2H3
InchiKey: WARDRXLFJRAMNM-UHFFFAOYSA-N
Formula: C10H21N
SMILES: CCCCCN1CCCC(C)C1
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	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1184.00		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=R221986&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

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