

N-(3'-Methylbutyl)pyrrolidine

Other names: N-(3-Methylbutyl)pyrrolidine
Inchi: InChI=1S/C9H19N/c1-9(2)5-8-10-6-3-4-7-10/h9H,3-8H2,1-2H3
InchiKey: VPXUTZPMWJIVMW-UHFFFAOYSA-N
Formula: C9H19N
SMILES: CC(C)CCN1CCCC1
Mol. weight [g/mol]: 141.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	2.128		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
ripol	1106.00		NIST Webbook
ripol	1116.00		NIST Webbook
ripol	1116.00		NIST Webbook
ripol	1106.00		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=R342642&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/73-372-8/N-3-Methylbutyl-pyrrolidine.pdf>

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