

5-methyl-N-isobutyl 3-pyrroline

Inchi: InChI=1S/C9H17N/c1-8(2)7-10-6-4-5-9(10)3/h4-5,8-9H,6-7H2,1-3H3
InchiKey: AQGPGTSPNDCWCK-UHFFFAOYSA-N
Formula: C9H17N
SMILES: CC(C)CN1CC=CC1C
Mol. weight [g/mol]: 139.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	1.903		Crippen Method
mcvol	132.490	ml/mol	McGowan Method
ripol	1237.00		NIST Webbook
ripol	1237.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314855&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
ripol: Polar retention indices

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