

2-methyl-6-butylpyraïne

Inchi: InChI=1S/C9H14N2/c1-3-4-5-9-7-10-6-8(2)11-9/h6-7H,3-5H2,1-2H3
InchiKey: UXSNPZYBZGYXMW-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: CCCCc1cncc(C)n1
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.128		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1120.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R219740&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

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