2-n-Propyl-1,2,3,4-tetrahydro-1-methylquinoline

Inchi: InChI=1S/C13H19N/c1-3-6-12-10-9-11-7-4-5-8-13(11)14(12)2/h4-5,7-8,12H,3,6,9-10H2,1
InchiKey: LRJFENJNBIDXQZ-UHFFFAOYSA-N
Formula: C13H19N
SMILES: CCCC1CCc2ccccc2N1C
Mol. weight [g/mol]: 189.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	3.238		Crippen Method
mcvol	169.390	ml/mol	McGowan Method
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398299&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.