

N-propyl-Octahydroindole

Inchi: InChI=1S/C11H21N/c1-2-8-12-9-7-10-5-3-4-6-11(10)12/h10-11H,2-9H2,1H3
InchiKey: WBYBVLUDSFJLEH-UHFFFAOYSA-N
Formula: C11H21N
SMILES: CCCN1CCC2CCCCC21
Mol. weight [g/mol]: 167.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.661		Crippen Method
mcvol	154.110	ml/mol	McGowan Method
rinpol	1317.00		NIST Webbook
rinpol	1300.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1477.00		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=R135385&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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