

# 1-propyl-1H-indole

**Inchi:** InChI=1S/C11H13N/c1-2-8-12-9-7-10-5-3-4-6-11(10)12/h3-7,9H,2,8H2,1H3  
**InchiKey:** LAAHPFCQVWTSIK-UHFFFAOYSA-N  
**Formula:** C11H13N  
**SMILES:** CCCn1ccc2ccccc21  
**Mol. weight [g/mol]:** 159.23  
**CAS:** 16885-94-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	3.051		Crippen Method
mcvol	136.910	ml/mol	McGowan Method
rinpol	1431.00		NIST Webbook
rinpol	1445.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2086.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16885942&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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  
**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices

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