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/ci990307l
Crippen Method: 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