

Indole-1-propionamide

Other names:	1H-indole-1-propionamide
Inchi:	InChI=1S/C11H12N2O/c12-11(14)6-8-13-7-5-9-3-1-2-4-10(9)13/h1-5,7H,6,8H2,(H2,12,14)
InchiKey:	VITGGSSBWKUFGR-UHFFFAOYSA-N
Formula:	C11H12N2O
SMILES:	NC(=O)CCn1ccc2ccccc21
Mol. weight [g/mol]:	188.23
CAS:	21017-50-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	1.517		Crippen Method
mcvol	148.460	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21017505&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

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<https://www.chemeo.com/cid/24-263-3/Indole-1-propionamide.pdf>

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