

Indole, 1-propionyl-

Other names:	1-(1-oxopropyl)-1H-indole
Inchi:	InChI=1S/C11H11NO/c1-2-11(13)12-8-7-9-5-3-4-6-10(9)12/h3-8H,2H2,1H3
InchiKey:	XBYKGSPCVQTMGF-UHFFFAOYSA-N
Formula:	C11H11NO
SMILES:	CCC(=O)n1ccc2ccccc21
Mol. weight [g/mol]:	173.21
CAS:	73747-53-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.691		Crippen Method
mcvol	138.480	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=C73747532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/77-186-1/Indole-1-propionyl.pdf>

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