

# Indole-1-carboxylic acid, ethyl ester

<b>Other names:</b>	ethyl 1H-indole-1-carboxylate
<b>Inchi:</b>	InChI=1S/C11H11NO2/c1-2-14-11(13)12-8-7-9-5-3-4-6-10(9)12/h3-8H,2H2,1H3
<b>InchiKey:</b>	OEXNQFWEJRSZBW-UHFFFAOYSA-N
<b>Formula:</b>	C11H11NO2
<b>SMILES:</b>	CCOC(=O)n1ccc2ccccc21
<b>Mol. weight [g/mol]:</b>	189.21
<b>CAS:</b>	13307-67-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.646		Crippen Method
mcvol	144.350	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13307670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13307670&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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