

# Ethyl 9H-pyrido(3,4-b)indole-3-carboxylate

<b>Other names:</b>	«beta»-Carboline-3-carboxylic acid ethyl ester Ethyl-«beta»-carboline-3-carboxylate Ethyl 9H-beta-carboline-3-carboxylate
<b>Inchi:</b>	InChI=1S/C14H12N2O2/c1-2-18-14(17)12-7-10-9-5-3-4-6-11(9)16-13(10)8-15-12/h3-8,10
<b>InchiKey:</b>	KOVRZNUMIKACTB-UHFFFAOYSA-N
<b>Formula:</b>	C14H12N2O2
<b>SMILES:</b>	CCOC(=O)c1cc2c(c[n1])[nH]c1cccc12
<b>Mol. weight [g/mol]:</b>	240.26
<b>CAS:</b>	74214-62-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	2.411		Crippen Method
mcvol	177.140	ml/mol	McGowan Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C74214623&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74214623&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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
<b>rinpol:</b>	Non-polar retention indices

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