

# Butanoic acid, 1H-indol-3-yl ester

<b>Other names:</b>	indol-3-yl butyrate
<b>Inchi:</b>	InChI=1S/C12H13NO2/c1-2-5-12(14)15-11-8-13-10-7-4-3-6-9(10)11/h3-4,6-8,13H,2,5H2
<b>InchiKey:</b>	DPUSLOQBAPOARC-UHFFFAOYSA-N
<b>Formula:</b>	C12H13NO2
<b>SMILES:</b>	CCCC(=O)Oc1c[nH]c2ccccc12
<b>Mol. weight [g/mol]:</b>	203.24
<b>CAS:</b>	4346-15-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.391		Crippen Method
mcvol	158.440	ml/mol	McGowan Method

## Sources

<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>
<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=C4346150&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4346150&amp;Units=SI</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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