

# Dimethyl indole-2,3-dicarboxylate

Other names:	Indole-2,3-dicarboxylic acid, dimethyl(ester)
Inchi:	InChI=1S/C12H11NO4/c1-16-11(14)9-7-5-3-4-6-8(7)13-10(9)12(15)17-2/h3-6,13H,1-2H3
InchiKey:	JNRXSMOJWKDVHC-UHFFFAOYSA-N
Formula:	C12H11NO4
SMILES:	COC(=O)c1[nH]c2ccccc2c1C(=O)OC
Mol. weight [g/mol]:	233.22
CAS:	54781-93-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	1.259		Crippen Method
mcvol	165.880	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54781930&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54781930&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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