

1H-Indole-3-acetic acid, methyl ester

Other names:	Indole-3-acetic acid, methyl ester «beta»-Indolylacetic acid methyl ester IAA Methyl ester Methyl «beta»-indoleacetate Methyl indole-3-acetate Methyl 3-indolylacetate Methyl «beta»-indolylacetate Indole-3-methyl acetate Methyl ester of 3-indoleacetic acid Methyl 1H-indole-3-acetate Methyl indol-3-ylacetate indole-3-acetic acid, Me Indoleacetic acid, methyl (1H-Indol-3-yl)-acetic acid methyl ester
Inchi:	InChI=1S/C11H11NO2/c1-14-11(13)6-8-7-12-10-5-3-2-4-9(8)10/h2-5,7,12H,6H2,1H3
InchiKey:	KTHADMMDGDNYQRX-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	COC(=O)Cc1c[nH]c2cccc12
Mol. weight [g/mol]:	189.21
CAS:	1912-33-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	1.401		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
rinpol	1854.30		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	306.59		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912330&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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