3-Indoleacrylic acid, methyl ester

Other names:	Methyl (2E)-3-(1H-indol-3-yl)acrylate
Inchi:	InChI=1S/C12H11NO2/c1-15-12(14)7-6-9-8-13-11-5-3-2-4-10(9)11/h2-8,13H,1H3/b7-6+
InchiKey:	JKVXFZPEUCTHQO-VOTSOKGWSA-N
Formula:	C12H11NO2
SMILES:	COC(=O)C=Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	201.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	1.872		Crippen Method
mcvol	154.140	ml/mol	McGowan Method
rinpol	2230.00		NIST Webbook
rinpol	2231.50		NIST Webbook
rinpol	2230.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333120&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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