

Ethyl indole-3-acrylate

Inchi:	InChI=1S/C13H13NO2/c1-2-16-13(15)8-7-10-9-14-12-6-4-3-5-11(10)12/h3-9,14H,2H2,1H
InchiKey:	OQJSITNIWIYWPU-BQYQJAHWSA-N
Formula:	C13H13NO2
SMILES:	CCOC(=O)C=Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	215.25
CAS:	15181-86-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	2.262		Crippen Method
mcvol	168.230	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15181869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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