

1H-Indole-2-carboxylic acid, 5-chloro-, ethyl ester

Other names:

Ethyl 5-chloroindole-2-carboxylate
Indole-2-carboxylic acid, 5-chloro-, ethyl ester
Ethyl 5-chloro-2-indolecarboxylate
Ethyl 5-chloro-1H-indole-2-carboxylate

Inchi:

InChI=1S/C11H10ClNO2/c1-2-15-11(14)10-6-7-5-8(12)3-4-9(7)13-10/h3-6,13H,2H2,1H3

InchiKey:

LWKIFKYHCJAIAB-UHFFFAOYSA-N

Formula:

C11H10ClNO2

SMILES:

CCOC(=O)c1cc2cc(Cl)ccc2[nH]1

Mol. weight [g/mol]:

223.66

CAS:

4792-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.516		Crippen Method
mcvol	156.590	ml/mol	McGowan Method
rinsol	1938.00		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=C4792670&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

rinsol:

Non-polar retention indices

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