

Ethyl 5-hydroxyindole-2-carboxylate

Other names:	1H-Indole-2-carboxylic acid, 5-hydroxy-, ethyl ester ethyl 5-hydroxy-1H-indole-2-carboxylate
Inchi:	InChI=1S/C11H11NO3/c1-2-15-11(14)10-6-7-5-8(13)3-4-9(7)12-10/h3-6,12-13H,2H2,1H1
InchiKey:	WANAXLMRGYGCP-UHFFFAOYSA-N
Formula:	C11H11NO3
SMILES:	CCOC(=O)c1cc2cc(O)ccc2[nH]1
Mol. weight [g/mol]:	205.21
CAS:	24985-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.568		Crippen Method
mcvol	150.220	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=C24985851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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