

Ethyl 5,6-dimethoxyindole-2-carboxylate

Other names:	1H-Indole-2-carboxylic acid, 5,6-dimethoxy-, ethyl ester ethyl 5,6-dimethoxy-1H-indole-2-carboxylate
Inchi:	InChI=1S/C13H15NO4/c1-4-18-13(15)10-5-8-6-11(16-2)12(17-3)7-9(8)14-10/h5-7,14H,4
InchiKey:	RBUSDPZPBBAKR-UHFFFAOYSA-N
Formula:	C13H15NO4
SMILES:	CCOC(=O)c1cc2cc(OC)c(OC)cc2[nH]1
Mol. weight [g/mol]:	249.26
CAS:	16382-18-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	1.880		Crippen Method
mcvol	184.270	ml/mol	McGowan Method

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=C16382186&Units=SI

Legend

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

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