

5-Methoxyindole-2-carboxylic acid

Other names:	1H-Indole-2-carboxylic acid, 5-methoxy- Indole-2-carboxylic acid, 5-methoxy- Acide methoxy-5 indole carboxylique-2 5-Methoxy-2-indolecarboxylic acid
Inchi:	InChI=1S/C10H9NO3/c1-14-7-2-3-8-6(4-7)5-9(11-8)10(12)13/h2-5,11H,1H3,(H,12,13)
InchiKey:	YEBJVSLNUMZXRJ-UHFFFAOYSA-N
Formula:	C10H9NO3
SMILES:	<chem>COc1ccc2[nH]c(C(=O)O)cc2c1</chem>
Mol. weight [g/mol]:	191.18
CAS:	4382-54-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.393		Crippen Method
mcvol	136.130	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=C4382541&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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