

1H-Indole-2-carboxylic acid, 1-methyl-

Other names:	Indole-2-carboxylic acid, 1-methyl- 1-Methylindole-2-carboxylic acid 1-Methyl-1H-indole-2-carboxylic acid 1-Methyl-2-indolecarboxylic acid
Inchi:	InChI=1S/C10H9NO2/c1-11-8-5-3-2-4-7(8)6-9(11)10(12)13/h2-6H,1H3,(H,12,13)
InchiKey:	MAHAMBLNIDMREX-UHFFFAOYSA-N
Formula:	C10H9NO2
SMILES:	<chem>Cn1c(C(=O)O)cc2ccccc21</chem>
Mol. weight [g/mol]:	175.18
CAS:	16136-58-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	1.876		Crippen Method
mcvol	130.260	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=C16136586&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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