

Indole-2-carboxylic acid

Other names:	1H-indole-2-carboxylic acid 2-Indolecarboxylic acid 2-carboxyindole 2-indolylformic acid indole-2-formic acid
Inchi:	InChI=1S/C9H7NO2/c11-9(12)8-5-6-3-1-2-4-7(6)10-8/h1-5,10H,(H,11,12)
InchiKey:	HCUARRIEZVDMPT-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	O=C(O)c1cc2ccccc2[nH]1
Mol. weight [g/mol]:	161.16
CAS:	1477-50-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.384		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
tf	483.10	K	Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives:	https://www.doi.org/10.1016/j.jct.2016.02.008
Solubilities of Indole-2-carboxylic Acid in Ten Different Pure Solvents from (278.15 to 360.15) K:	https://www.doi.org/10.1021/je400813d

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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