

# Indole-2-carboxylic acid

<b>Other names:</b>	1H-indole-2-carboxylic acid 2-Indolecarboxylic acid 2-carboxyindole 2-indolylformic acid indole-2-formic acid
<b>Inchi:</b>	InChI=1S/C9H7NO2/c11-9(12)8-5-6-3-1-2-4-7(6)10-8/h1-5,10H,(H,11,12)
<b>InchiKey:</b>	HCUARRIEZVDMPT-UHFFFAOYSA-N
<b>Formula:</b>	C9H7NO2
<b>SMILES:</b>	O=C(O)c1cc2cccc2[nH]1
<b>Mol. weight [g/mol]:</b>	161.16
<b>CAS:</b>	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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477505&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477505&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Experimental and computational thermochemical study of benzofuran, Benzothiophene and Indole Derivatives:</b>	<a href="https://www.doi.org/10.1016/j.jct.2016.02.008">https://www.doi.org/10.1016/j.jct.2016.02.008</a>
<b>Solubilities of Indole-2-carboxylic Acid</b>	<a href="https://www.doi.org/10.1021/je400813d">https://www.doi.org/10.1021/je400813d</a>
<b>McGowan Method</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>(278.15 to 360.15) K:</b>	

# 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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