

# Indole-3-acetaldehyde

<b>Other names:</b>	Tryptaldehyde
<b>Inchi:</b>	InChI=1S/C10H9NO/c12-6-5-8-7-11-10-4-2-1-3-9(8)10/h1-4,6-7,11H,5H2
<b>InchiKey:</b>	WHOOUMGHGSPMGR-UHFFFAOYSA-N
<b>Formula:</b>	C10H9NO
<b>SMILES:</b>	O=CCc1c[nH]c2ccccc12
<b>Mol. weight [g/mol]:</b>	159.18
<b>CAS:</b>	2591-98-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	1.427		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
rinpola	1713.20		NIST Webbook

## Sources

<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>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2591982&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2591982&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpola:</b>	Non-polar retention indices

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