

# N-Acetylindole

<b>Other names:</b>	1H-Indole, 1-acetyl- Indole, 1-acetyl- 1-Acetyl-1H-indole 1-Acetylindole Acetylindole
<b>Inchi:</b>	InChI=1S/C10H9NO/c1-8(12)11-7-6-9-4-2-3-5-10(9)11/h2-7H,1H3
<b>InchiKey:</b>	UUCUQJHYUPXDHN-UHFFFAOYSA-N
<b>Formula:</b>	C10H9NO
<b>SMILES:</b>	CC(=O)n1ccc2ccccc21
<b>Mol. weight [g/mol]:</b>	159.18
<b>CAS:</b>	576-15-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	2.301		Crippen Method
mvol	124.390	ml/mol	McGowan Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2481.00		NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.70	K	1.90	NIST Webbook

## Sources

<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=C576158&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C576158&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure

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