

# N-Acetyl-3-methylindole

**Inchi:** InChI=1S/C11H11NO/c1-8-7-12(9(2)13)11-6-4-3-5-10(8)11/h3-7H,1-2H3  
**InchiKey:** BWMWADPREVTFDJ-UHFFFAOYSA-N  
**Formula:** C11H11NO  
**SMILES:** CC(=O)n1cc(C)c2ccccc21  
**Mol. weight [g/mol]:** 173.21  
**CAS:** 23543-66-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	2.610		Crippen Method
mcvol	138.480	ml/mol	McGowan Method
rinpol	1643.00		NIST Webbook
ripol	2558.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2558.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23543660&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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