

# N-Acetyl-2,3-dimethyl-indole

**Inchi:** InChI=1S/C12H13NO/c1-8-9(2)13(10(3)14)12-7-5-4-6-11(8)12/h4-7H,1-3H3  
**InchiKey:** UCHBCCUSCVVGCY-UHFFFAOYSA-N  
**Formula:** C12H13NO  
**SMILES:** CC(=O)n1c(C)c(C)c2ccccc21  
**Mol. weight [g/mol]:** 187.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	2.918		Crippen Method
mcvol	152.570	ml/mol	McGowan Method
rinpol	1723.00		NIST Webbook
ripol	2595.00		NIST Webbook
ripol	2654.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R135276&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## 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

Latest version available from:

<https://www.cheméo.com/cid/94-181-7/N-Acetyl-2-3-dimethyl-indole.pdf>

Generated by Cheméo on 2024-04-25 06:24:31.469688251 +0000 UTC m=+16315520.390265563.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.