# 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/ci990307l
**Crippen Method:** 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

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