N-Acetyl-2-methyl-indole

Inchi: InChI=1S/C11H11NO/c1-8-7-10-5-3-4-6-11(10)12(8)9(2)13/h3-7H,1-2H3
InchiKey: MQKDFUDWMKTCNQ-UHFFFAOYSA-N
Formula: C11H11NO
SMILES: CC(=O)n1c(C)cc2ccccc21
Mol. weight [g/mol]: 173.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	2.610		Crippen Method
mcvol	138.480	ml/mol	McGowan Method
ripol	2483.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R135281&Units=SI

Legend

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