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
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/ci990307l

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