

1H-Indole-3-ethanol, acetate (ester)

Other names: 3-(2-Hydroxyethyl)indole, O-acetyl-
Inchi: InChI=1S/C12H13NO2/c1-9(14)15-7-6-10-8-13-12-5-3-2-4-11(10)12/h2-5,8,13H,6-7H2,1
InchiKey: KAWBLROQFPLJEU-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: CC(=O)OCCc1c[nH]c2ccccc12
Mol. weight [g/mol]: 203.24
CAS: 13137-14-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	1.792		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
rinpol	1926.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1926.00		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=C13137149&Units=SI>

Legend

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

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