

Ethanone, 1-(1H-indol-3-yl)-

Other names:	Ketone, indol-3-yl methyl 3-Acetyl-1H-indole 3-Acetylindole 3-Indolyl methyl ketone Acetyl-3-indole indol-3-yl methyl ketone
Inchi:	InChI=1S/C10H9NO/c1-7(12)9-6-11-10-5-3-2-4-8(9)10/h2-6,11H,1H3
InchiKey:	VUIMBZIZZFSQEE-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	CC(=O)c1c[nH]c2ccccc12
Mol. weight [g/mol]:	159.18
CAS:	703-80-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	1.889		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C703800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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