1,3-Diacetylindole

Other names:	1H-Indole, 1,3-diacetyl- 1,3-Diacetylindol N,3-diacetyl-indole 1,3-diacetyl-1H-indole
Inchi:	InChI=1S/C12H11NO2/c1-8(14)11-7-13(9(2)15)12-6-4-3-5-10(11)12/h3-7H,1-2H3
InchiKey:	STUZJORZRZCLRI-UHFFFAOYSA-N
Formula:	C12H11NO2
SMILES:	CC(=O)c1cn(C(C)=O)c2ccccc12
Mol. weight [g/mol]:	201.22
CAS:	17537-64-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	2.504		Crippen Method
mcvol	154.140	ml/mol	McGowan Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		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=C17537643&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