Imidazole, 2,3-dihydro-1-methyl-2-acetylimino-3-acetyl-4acet

Inchi: InChI=1S/C10H13N3O4/c1-6(14)11-10-12(4)5-9(17-8(3)16)13(10)7(2)15/h5H,1-4H3
InchiKey: XQQGTGGNNCOQBW-UHFFFAOYSA-N
Formula: C10H13N3O4
SMILES: CC(=O)N=c1n(C)cc(OC(C)=O)n1C(C)=O
Mol. weight [g/mol]: 239.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	-0.141		Crippen Method
mcvol	172.820	ml/mol	McGowan Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374347&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.