2H-Pyran-2-one, 3-acetyl-4-hydroxy-6-methyl-

Other names: 3-acetyl-4-hydroxy-6-methyl-2H-pyran-2-one
Inchi: InChI=1S/C8H8O4/c1-4-3-6(10)7(5(2)9)8(11)12-4/h3,10H,1-2H3
InchiKey: PKLPQOJFHFGVBS-UHFFFAOYSA-N
Formula: C8H8O4
SMILES: CC(=O)c1c(O)cc(C)oc1=O
Mol. weight [g/mol]: 168.15
CAS: 771-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	0.856		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C771039&Units=SI
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

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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