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

Physical Properties

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C771039&Units=SI

Legend

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.