

3-Acetoxy-2-methyl-pyran-4-one

Other names: 3-Hydroxy-2-methyl-pyran-4-one acetate
Inchi: InChI=1S/C8H8O4/c1-5-8(12-6(2)9)7(10)3-4-11-5/h3-4H,1-2H3
InchiKey: NRQULFRLDJKNGP-UHFFFAOYSA-N
Formula: C8H8O4
SMILES: CC(=O)Oc1c(C)occc1=O
Mol. weight [g/mol]: 168.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	0.874		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook

Sources

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=U373049&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/41-495-7/3-Acetoxy-2-methyl-pyran-4-one.pdf>

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