

# (Z)-3-Hydroxy-3-methyl-1-((7-oxo-7H-furo[3,2-g]chromen-2-yl)oxy)but-2-enoate

InChI: InChI=1S/C21H22O7/c1-5-12(2)20(23)27-15(21(3,4)24)11-26-19-17-14(8-9-25-17)10-13  
InChIKey: VJWXQSFKTVUEFY-XGICHPGQSA-N  
Formula: C21H22O7  
SMILES: CC=C(C)C(=O)OC(COc1c2occc2cc2ccc(=O)oc12)C(C)(C)O  
Mol. weight [g/mol]: 386.40  
CAS: 27542-14-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.06		Crippen Method
logp	3.567		Crippen Method
mcvol	280.860	ml/mol	McGowan Method
rinpol	3002.00		NIST Webbook
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## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C27542149&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

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