(Z)-3-Hydroxy-3-methyl-1-((7-oxo-7H-furo[3,2-g]ch
2-methylbut-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: VJVXQSFKTVUEFY-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
rinpol	3002.00		NIST Webbook

Sources

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
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