(R,Z)-3-Hydroxy-3-methyl-1-((7-oxo-7H-furo[3,2-g]
2-methylbut-2-enoate

Inchi:	InChI=1S/C21H22O7/c1-5-12(2)20(23)28-17(21(3,4)24)11-26-19-13-6-7-18(22)27-16(13)
InchiKey:	WXULKGXQMWVWMP-OMLDUKLJSA-N
Formula:	C21H22O7
SMILES:	CC=C(C)C(=O)OC(COc1c2ccoc2cc2oc(=O)ccc12)C(C)(C)O
Mol. weight [g/mol]:	386.40
CAS:	642-08-0

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	3048.80		NIST Webbook
rinpol	3048.80		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=C642080&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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