(S,Z)-3-Hydroxy-1-((9-methoxy-7-oxo-7H-furo[3,2-g
2-methylbut-2-enoate

Inchi: InChI=1S/C22H24O8/c1-6-12(2)21(24)29-15(22(3,4)25)11-28-17-13-7-8-16(23)30-19(13)
InchiKey: VTMREZQNDKWTII-GIXCSOPHSA-N
Formula: C22H24O8
SMILES: CC=C(C)C(=O)OC(COc1c2ccoc2c(OC)c2oc(=O)ccc12)C(C)(C)O
Mol. weight [g/mol]: 416.42
CAS: 116988-91-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.18		Crippen Method
logp	3.575		Crippen Method
mcvol	300.820	ml/mol	McGowan Method
rinpol	3170.40		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=C116988911&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
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.