(S)-8,8-Dimethyl-2-oxo-7,8-dihydro-2H,6H-pyrano(
3-methyl-2-butenoate

Other names: 8,8-Dimethyl-2-oxo-7,8-dihydro-2H,6H-pyrano[3,2-g]chromen-7-yl 3-methyl-2-butenoate, (S)-
Decursin

Inchi: InChI=1S/C19H20O5/c1-11(2)7-18(21)23-16-9-13-8-12-5-6-17(20)22-14(12)10-15(13)24

InchiKey: CUKSFECWKQBVED-UHFFFAOYSA-N

Formula: C19H20O5

SMILES: CC(C)=CC(=O)OC1Cc2cc3ccc(=O)oc3cc2OC1(C)C

Mol. weight [g/mol]: 328.36

CAS: 5928-25-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.12		Crippen Method
logp	3.384		Crippen Method
mcvol	245.240	ml/mol	McGowan Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
rinpol	2792.00		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=C5928256&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