Benzo[1,2-b:5,4-b']difuran-4,8-dione, 2,3-dihydro-5-methyl-2-(1-methylethenyl)-, (-)-

Other names: Benzo(1,2-b:5,4-b')difuran-4,8-dione, 2,3-dihydro-2-isopropenyl-5-methyl-, (-)-
Dihydrocyperaquinone
(-)-2,3-Dihydro-2-isopropenyl-5-methylbenzo(1,2-b:5,4-b')difuran-4,8-dione

Inchi: InChI=1S/C14H12O4/c1-6(2)9-4-8-11(15)10-7(3)5-17-14(10)12(16)13(8)18-9/h5,9H,1,4H

InchiKey: NBEKXDAUYUYRQM-UHFFFAOYSA-N

Formula: C14H12O4

SMILES: C=C(C)C1CC2=C(O1)C(=O)c1occ(C)c1C2=O

Mol. weight [g/mol]: 244.24

CAS: 27304-02-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.29		Crippen Method
logp	2.586		Crippen Method
mcvol	173.220	ml/mol	McGowan Method

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=C27304025&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