

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:	<chem>C=C(C)C1CC2=C(O1)C(=O)c1occ(C)c1C2=O</chem>
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

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