4-([(2E)-3,7-dimethyl-2,6-octadienyl]oxy)-7h-furo[3

Inchi: InChI=1S/C21H22O4/c1-14(2)5-4-6-15(3)9-11-24-21-16-7-8-20(22)25-19(16)13-18-17(21
InchiKey: DBMJZOMNXBSRED-OQLLNIDSSA-N
Formula: C21H22O4
SMILES: CC(C)=CCCC(C)=CCOc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.56		Crippen Method
logp	5.611		Crippen Method
mcvol	263.250	ml/mol	McGowan Method

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=B6007553&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume