2-Furoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C15H18O3/c1-11(2)7-8-13(10-12(3)4)18-15(16)14-6-5-9-17-14/h5-6,9,12-13H,
InchiKey: KYWKCTFRHIELIT-UHFFFAOYSA-N
Formula: C15H18O3
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccco1
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.73		Crippen Method
logp	3.431		Crippen Method
mcvol	203.160	ml/mol	McGowan Method
rinpol	1633.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299238&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices