Information about the retrosynthesis

Created On: 2019-12-13T18:04:48.005000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C(C)1=CCCC(C)2CC/C(=C(/C)\C)/CC12
MSSR: 3
FAP: 0.65
MRP: 10
SbP: 1
Available smiles:
Exclude smiles: C(C)1=CCCC(C)2CC/C(=C(/C)\C)/CC12
Exclude substructures:

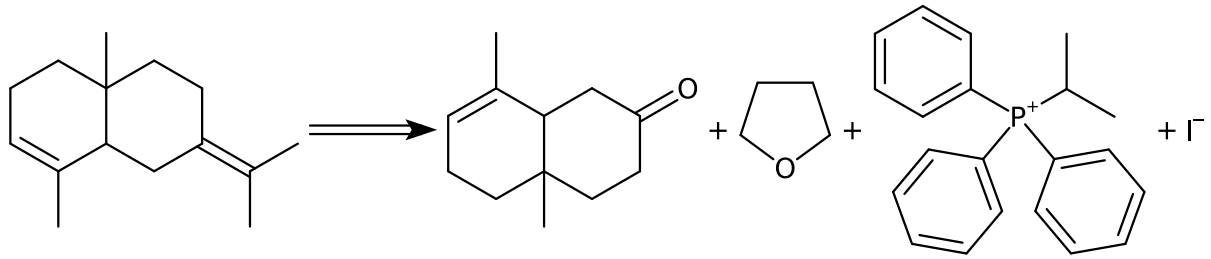
Sequence 0, Confidence: 0.978

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

Step 1

Type: Wittig olefination, Confidence: 0.994

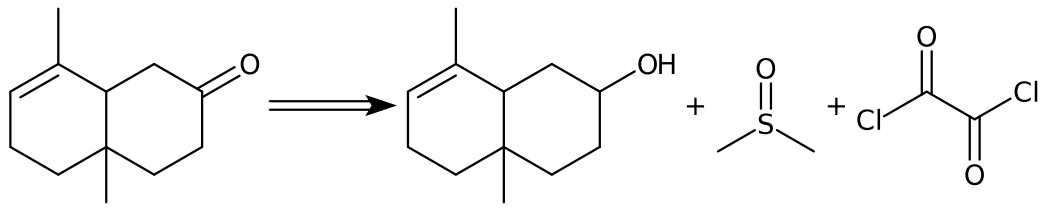
CC1=CCCC2(C)CCC(=O)CC12.C1CCOC1.CC(C)[P+](c1ccccc1)(c1ccccc1)c1ccccc1.[I-]>>CC1=CCCC2(C)CCC(=C(C)C)CC12



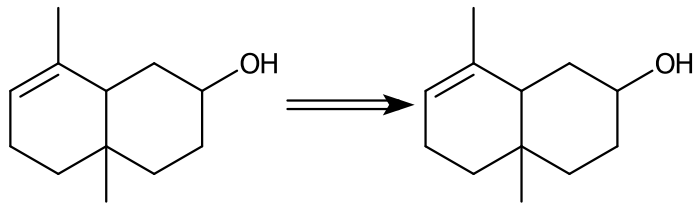
Step 2

Type: Ketone Swern oxidation, Confidence: 0.984

CC1=CCCC2(C)CCC(O)CC12.CS(C)=O.O=C(Cl)C(=O)Cl>>CC1=CCCC2(C)CCC(=O)CC12



Step 3

Type: Undefined, Confidence: 0.0

CC1=CCCC2(C)CCC(O)CC12>>CC1=CCCC2(C)CCC(O)CC12