Information about the retrosynthesis

Created On: 2019-12-13T18:03:59.247000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1/C(=C(/C)\C)/CCC(C)2CCCC(=C)C12
MSSR: 3
FAP: 0.65
MRP: 10
SbP: 1
Available smiles:
Exclude smiles: C1/C(=C(/C)\C)/CCC(C)2CCCC(=C)C12
Exclude substructures:

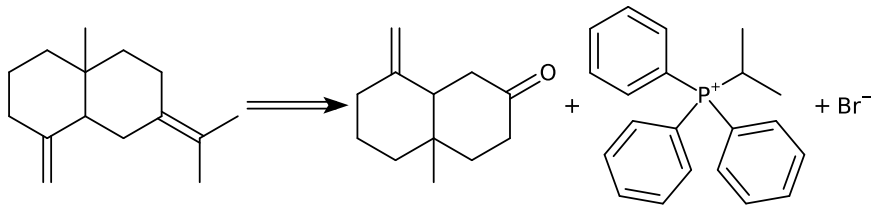
Sequence 0, Confidence: 0.808

Metadata:
Warnings: The retrosynthesis did not complete. Try increasing MSSR.

Step 1

Type: Wittig olefination, Confidence: 0.861

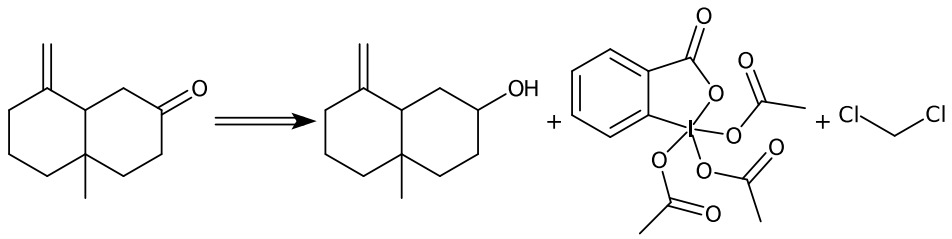
C=C1CCCC2(C)CCC(=O)CC12.CC(C)[P+](c1ccccc1)(c1ccccc1)c1ccccc1.[Br-]>>C=C1CCCC2(C)CCC(=C(C)C)CC12



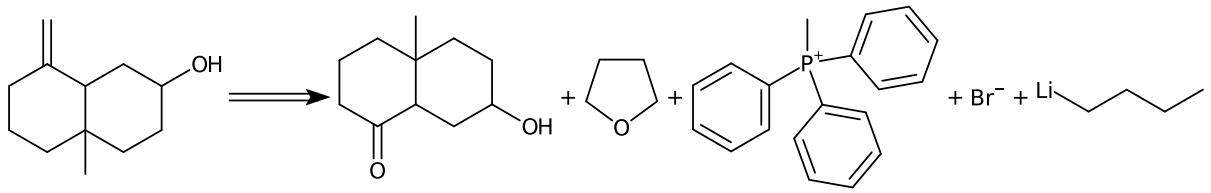
Step 2

Type: Ketone Dess-Martin oxidation, Confidence: 0.974

C=C1CCCC2(C)CCC(O)CC12.CC(=O)OI1(OC(C)=O)(OC(C)=O)OC(=O)c2ccccc21.ClCCl>>C=C1CCCC2(C)CCC(=O)CC12



Step 3

Type: Wittig olefination, Confidence: 0.964

CC12CCCC(=O)C1CC(O)CC2.C1CCOC1.C[P+](c1ccccc1)(c1ccccc1)c1ccccc1.[Br-].[Li]CCCC>>C=C1CCCC2(C)CCC(O)CC12