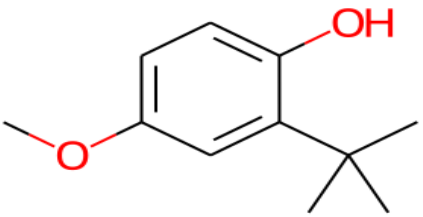
VERA: Similarity and Grouping:

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

Molecule Input:



TotGroups: 7

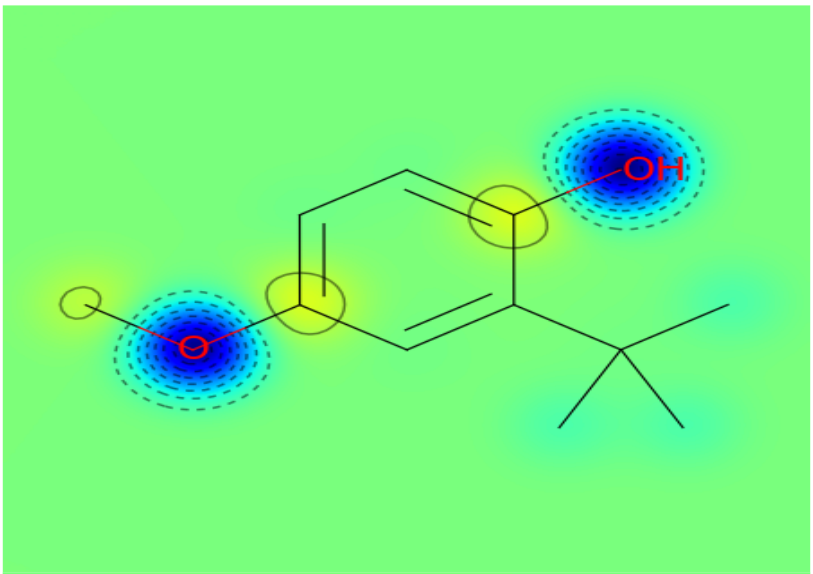
['methoxy', 'phenol', 'phenol_noOrthoHbond', 'Ar_OR', 'Ar_R', 'op_diphenolo_OR', 'CC4']

LogP: 2.698
MaxPartialCharge: 0.119
MinPartialCharge: -0.508
NumHAcceptors: 2
NumHDonors: 1
NumRotatableBonds: 1
NumAliphaticRings: 0
NumAromaticCarbocycles: 1
NumAromaticHeterocycles: 0
NumAromaticRings: 1
ExactMolWt: 180.115

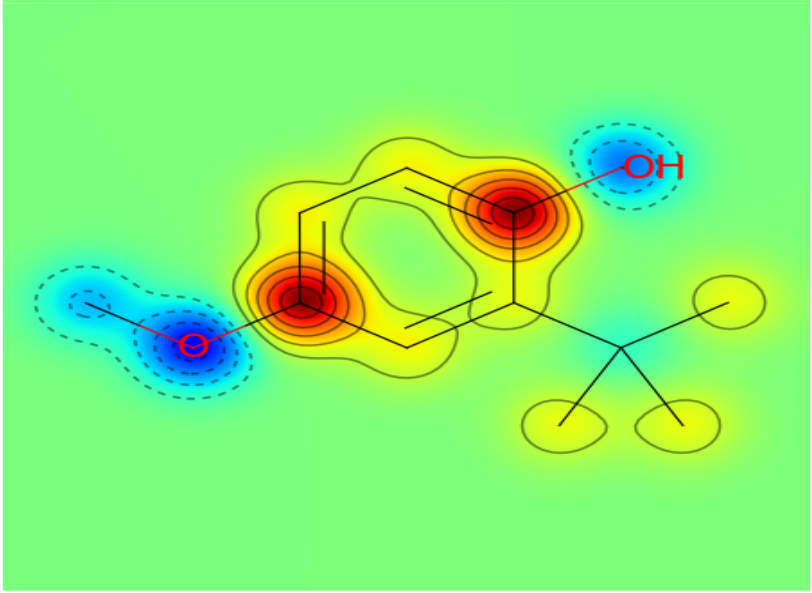
Experimental Value is known: Active

Prediction: equivocal2.0

GasteigerCharges:



CrippenContribs:



Molecules with the highest group similarity

1) SMILES: COc1ccc(O)c(C(C)(C)C)c1

Class: Active

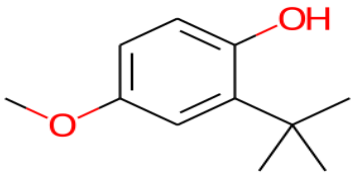
SimilarityVega: 1.0

SimilarityGrouping: 1.0

Grp_Similarity_Mean: 1.0

Groups in common: 9

TotGroups 9



GROUPS:
methoxy Stat: Neutro
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
Ar_OR Stat: Neutro
Ar_R Stat: Neutro
op_diphenolo_OR Stat: Neutro
CC4 Stat: Neutro
Alerts: []

2) SMILES: Cc1c(C)c2c(c(C)c1O)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2

Class: NON-Active

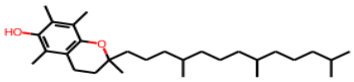
SimilarityVega: 0.684

SimilarityGrouping: 0.91

Grp_Similarity_Mean: 0.797

Groups in common: 8

TotGroups 11



GROUPS:
bicyclic Stat: Neutro
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
benzCH2 Stat: Neutro
Ar_OR Stat: Neutro
Ar_R Stat: Neutro
op_diphenolo_OR Stat: Neutro
CC4 Stat: Neutro
Alerts: []

3) SMILES: CC(C)(C)c1cc(O)ccc1O

Class: NON-Active

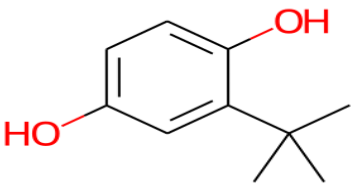
SimilarityVega: 0.948

SimilarityGrouping: 0.851

Grp_Similarity_Mean: 0.9

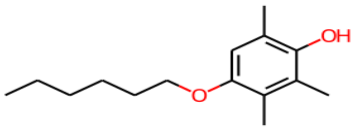
Groups in common: 7

TotGroups 10

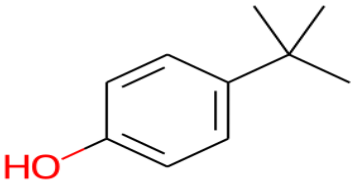


GROUPS:
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
biphenol Stat: Neutro
Ar_R Stat: Neutro
op_diphenolo_OR Stat: Neutro
CC4 Stat: Neutro
Alerts: []

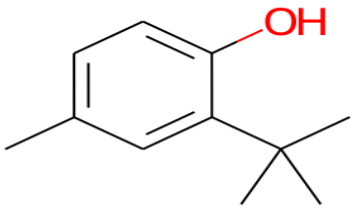
4) SMILES: CCCCCCOc1cc(C)c(O)c(C)c1C
Class: NON-Active
SimilarityVega: 0.842
SimilarityGrouping: 0.843
Grp_Similarity_Mean: 0.842
Groups in common: 7
TotGroups 11
GROUPS:
aryl_methyl Stat: Neutro
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
unbrch_alkane Stat: Neutro
Ar_OR Stat: Neutro
Ar_R Stat: Neutro
op_diphenolo_OR Stat: Neutro
Alerts: []



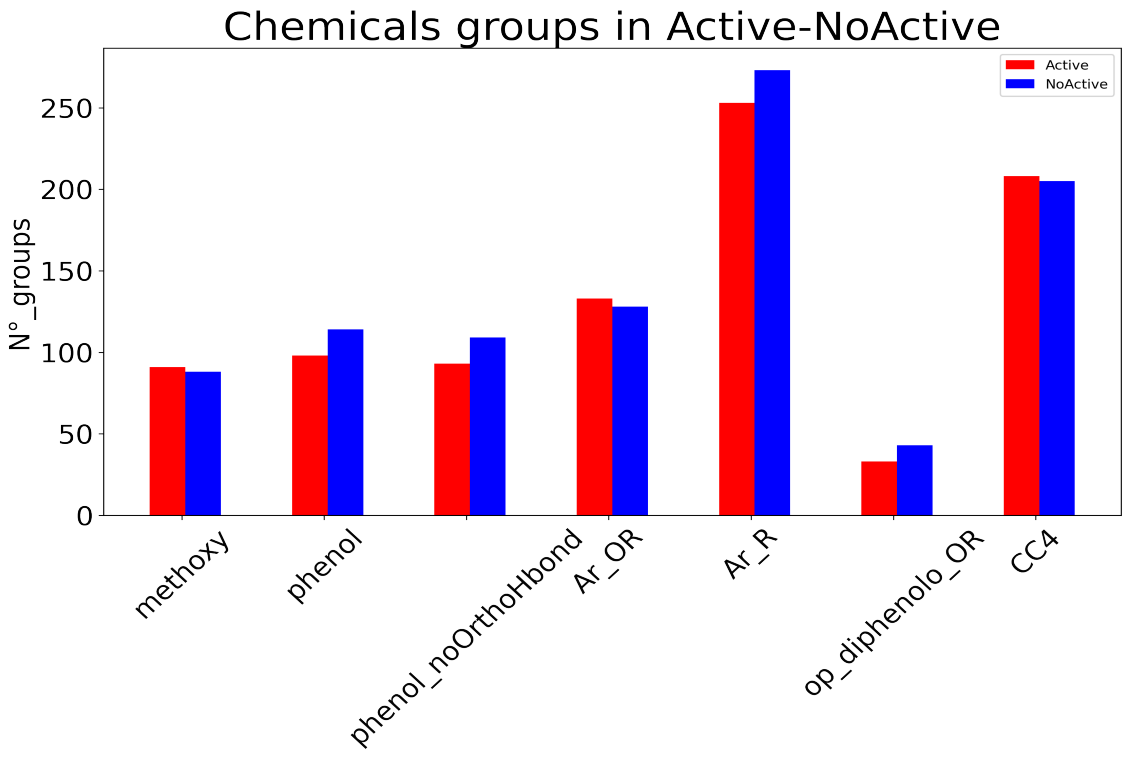
5) SMILES: CC(C)(C)c1ccc(O)cc1
Class: NON-Active
SimilarityVega: 0.875
SimilarityGrouping: 0.833
Grp_Similarity_Mean: 0.854
Groups in common: 6
TotGroups 6
GROUPS:
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
Ar_R Stat: Neutro
CC4 Stat: Neutro
Alerts: []



6) SMILES: Cc1ccc(O)c(C(C)(C)C)c1
Class: NON-Active
SimilarityVega: 0.892
SimilarityGrouping: 0.802
Grp_Similarity_Mean: 0.847
Groups in common: 6
TotGroups 8
GROUPS:
aryl_methyl Stat: Neutro
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
Ar_R Stat: Neutro
CC4 Stat: Neutro
Alerts: []



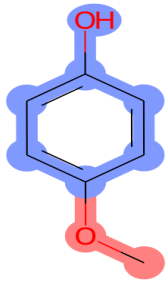
Molecule Input: Bar Chart for groups in dataset find in target



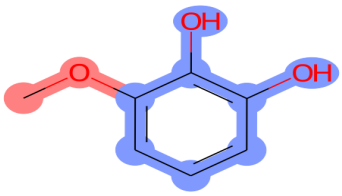
Reasoning

Ortogonal Research based on copresence of group with high prevalence methoxy and GRP phenol

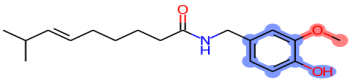
Smile: COc1ccc(O)cc1
Class: Active
Similarity: 0.849



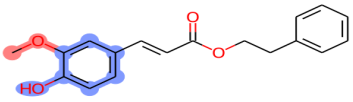
Smile: COc1cccc(O)c1O
Class: Active
Similarity: 0.807



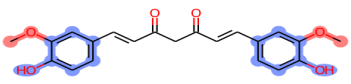
Smile: COc1cc(CNC(=O)CCCCC=CC(C)C)ccc1O
Class: Active
Similarity: 0.73



Smile: COc1cc(C=CC(=O)OCCc2ccccc2)ccc1O
Class: NON-Active
Similarity: 0.718



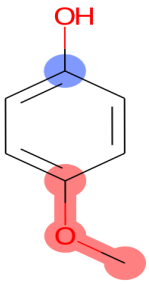
Smile:
COc1cc(C=CC(=O)CC(=O)C=Cc2ccc(O)c(OC)c2)ccc1O
Class: NON-Active
Similarity: 0.656



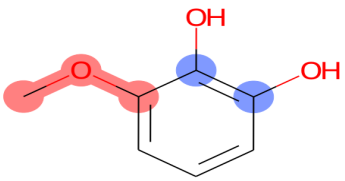
Reasoning

Ortogonal Research based on copresence of group with high prevalence methoxy and GRP phenol_noOrthoHbond

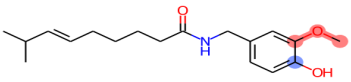
Smile: COc1ccc(O)cc1
Class: Active
Similarity: 0.849



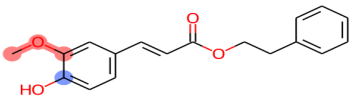
Smile: COc1cccc(O)c1O
Class: Active
Similarity: 0.807



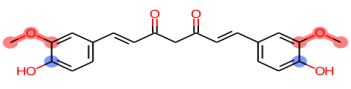
Smile: COc1cc(CNC(=O)CCCCC=CC(C)C)ccc1O
Class: Active
Similarity: 0.73



Smile: COc1cc(C=CC(=O)OCCc2ccccc2)ccc1O
Class: NON-Active
Similarity: 0.718



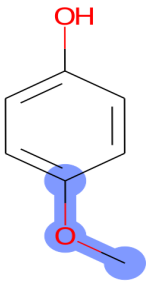
Smile:
COc1cc(C=CC(=O)CC(=O)C=Cc2ccc(O)c(OC)c2)ccc1O
Class: NON-Active
Similarity: 0.656



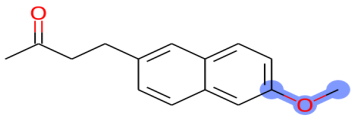
Reasoning

Ortogonal Research based on copresence of group with high prevalence methoxy and GRP Ar_OR

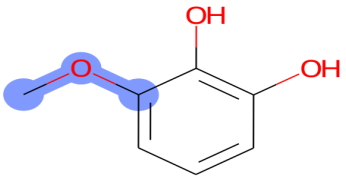
Smile: COc1ccc(O)cc1
Class: Active
Similarity: 0.849



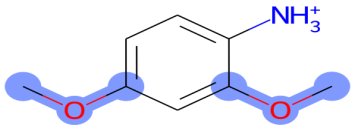
Smile: COc1ccc2cc(CCC(C)=O)ccc2c1
Class: NON-Active
Similarity: 0.833



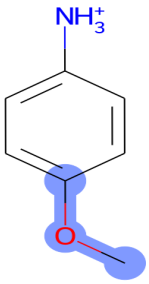
Smile: COc1cccc(O)c1O
Class: Active
Similarity: 0.807



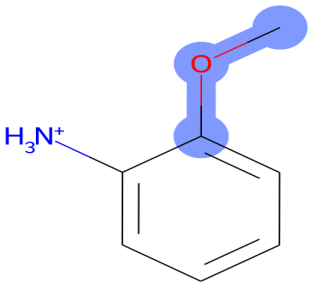
Smile: COc1ccc([NH3+])c(OC)c1
Class: NON-Active
Similarity: 0.806



Smile: COc1ccc([NH3+])cc1
Class: NON-Active
Similarity: 0.793



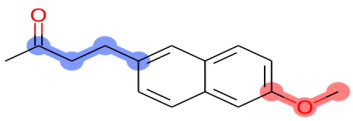
Smile: COc1ccccc1[NH3+]
Class: Active
Similarity: 0.79



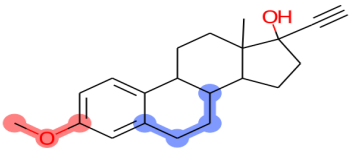
Reasoning

Ortogonal Research based on copresence of group with high prevalence methoxy and GRP Ar_R

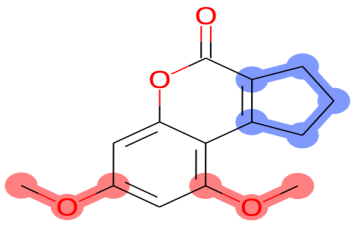
Smile: COc1ccc2cc(CCC(C)=O)ccc2c1
Class: NON-Active
Similarity: 0.833



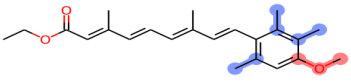
Smile: C#CC1(O)CCC2C3CCc4cc(OC)ccc4C3CCC21C
Class: Active
Similarity: 0.754



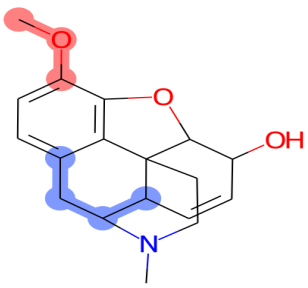
Smile: COc1cc(OC)c2c3c(c(=O)oc2c1)CCC3
Class: NON-Active
Similarity: 0.7030000000000001



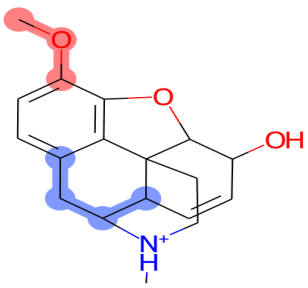
Smile: CCOC(=O)C=C(C)C=CC=C(C)C=Cc1c(C)cc(OC)c(C)c1C
Class: NON-Active
Similarity: 0.6930000000000001



Smile: COc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Class: NON-Active
Similarity: 0.664



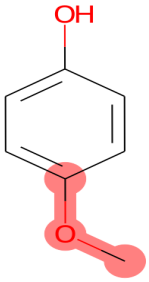
Smile: COc1ccc2c3c1OC1C(O)C=CC4C(C2)[NH+](C)CCC341
Class: NON-Active
Similarity: 0.66



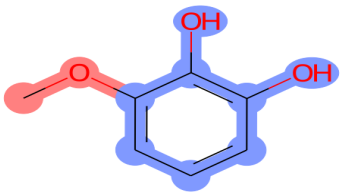
Reasoning

Ortogonal Research based on copresence of group with high prevalence methoxy and GRP op_diphenolo_OR

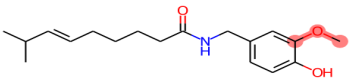
Smile: COc1ccc(O)cc1
Class: Active
Similarity: 0.849



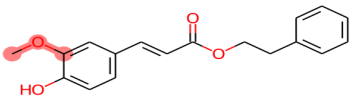
Smile: COc1cccc(O)c1O
Class: Active
Similarity: 0.807



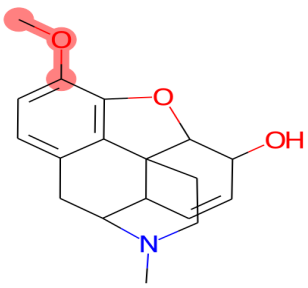
Smile: COc1cc(CNC(=O)CCCCC=CC(C)C)ccc1O
Class: Active
Similarity: 0.73



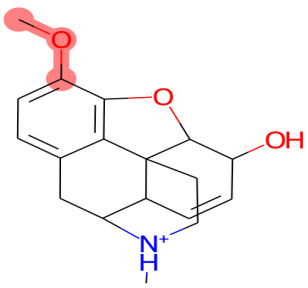
Smile: COc1cc(C=CC(=O)OCCc2ccccc2)ccc1O
Class: NON-Active
Similarity: 0.718



Smile: COc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Class: NON-Active
Similarity: 0.664



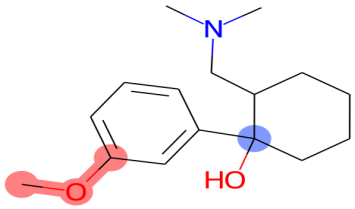
Smile:
COc1ccc2c3c1OC1C(O)C=CC4C(C2)[NH+](C)CCC341
Class: NON-Active
Similarity: 0.66



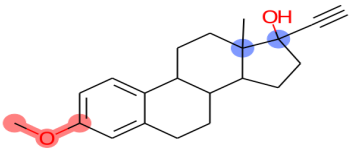
Reasoning

Ortogonal Research based on copresence of group with high prevalence methoxy and GRP CC4

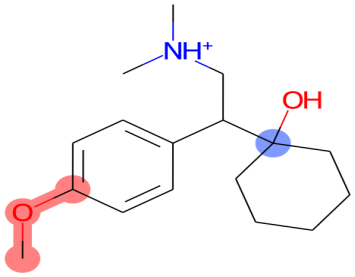
Smile: COc1cccc(C2(O)CCCCC2CN(C)C)c1
Class: NON-Active
Similarity: 0.76



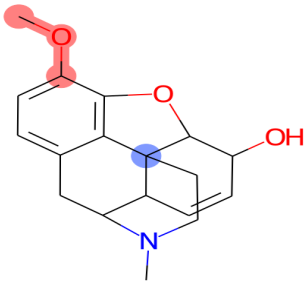
Smile: C#CC1(O)CCC2C3CCc4cc(OC)ccc4C3CCC21C
Class: Active
Similarity: 0.754



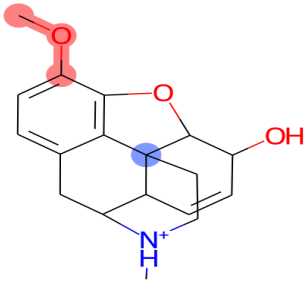
Smile: COc1ccc(C(C[NH+](C)C)C2(O)CCCCC2)cc1
Class: NON-Active
Similarity: 0.731



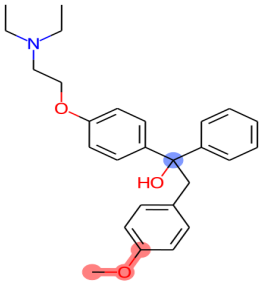
Smile: COc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Class: NON-Active
Similarity: 0.664



Smile:
COc1ccc2c3c1OC1C(O)C=CC4C(C2)[NH+](C)CCC341
Class: NON-Active
Similarity: 0.66

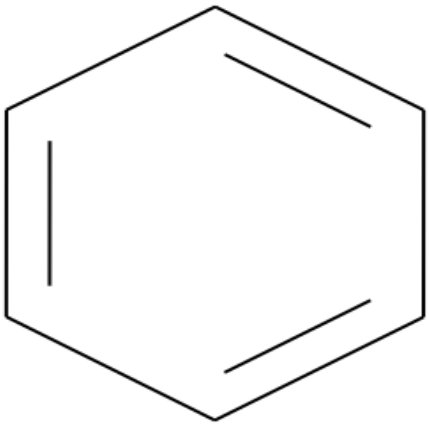


Smile:
CCN(CC)CCOc1ccc(C(O)(Cc2ccc(OC)cc2)c2ccccc2)cc1
Class: NON-Active
Similarity: 0.658

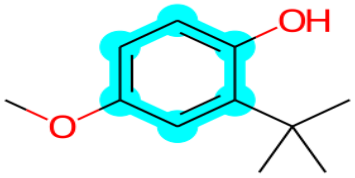


Scaffold

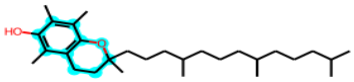
Scaffold analysis



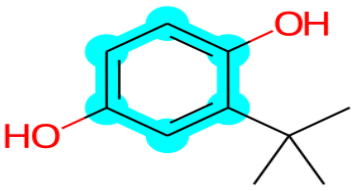
Smile: COc1ccc(O)c(C(C)(C)C)c1
Class: Active
Similarity: 1.0



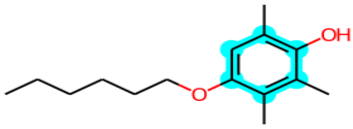
Smile: Cc1c(C)c2c(c(C)c1O)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Class: NON-Active
Similarity: 0.684



Smile: CC(C)(C)c1cc(O)ccc1O
Class: NON-Active
Similarity: 0.948



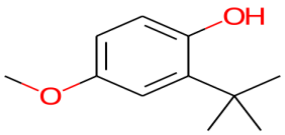
Smile: CCCCCCOc1cc(C)c(O)c(C)c1C
Class: NON-Active
Similarity: 0.842



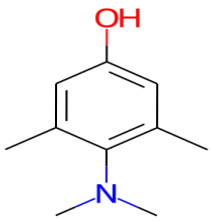
Descriptors

Calculator Similarity descriptor

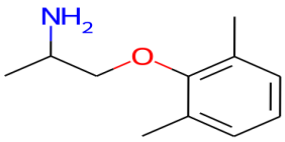
Smile: COc1ccc(O)c(C(C)(C)C)c1
Class: Active
DistanceCityBlock: 0.0
LogP:2.6983000000000006
MW: 180.115029752



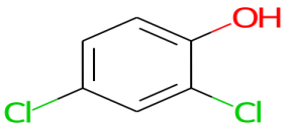
Smile: Cc1cc(O)cc(C)c1N(C)C
Class: NON-Active
DistanceCityBlock: 0.648
LogP:2.0750399999999996
MW: 165.1153641



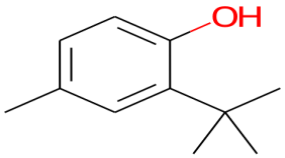
Smile: Cc1cccc(C)c1OCC(C)N
Class: NON-Active
DistanceCityBlock: 1.377
LogP:2.0294399999999997
MW: 179.131014164



Smile: Oc1ccc(Cl)cc1Cl
Class: NON-Active
DistanceCityBlock: 1.492
LogP:2.699
MW: 161.963920108



Smile: Cc1ccc(O)c(C(C)(C)C)c1
Class: NON-Active
DistanceCityBlock: 1.522
LogP:2.998120000000001
MW: 164.120115132



Smile: CC(C)(C)c1ccc(O)cc1
Class: NON-Active
DistanceCityBlock: 1.554
LogP:2.689700000000001
MW: 150.104465068