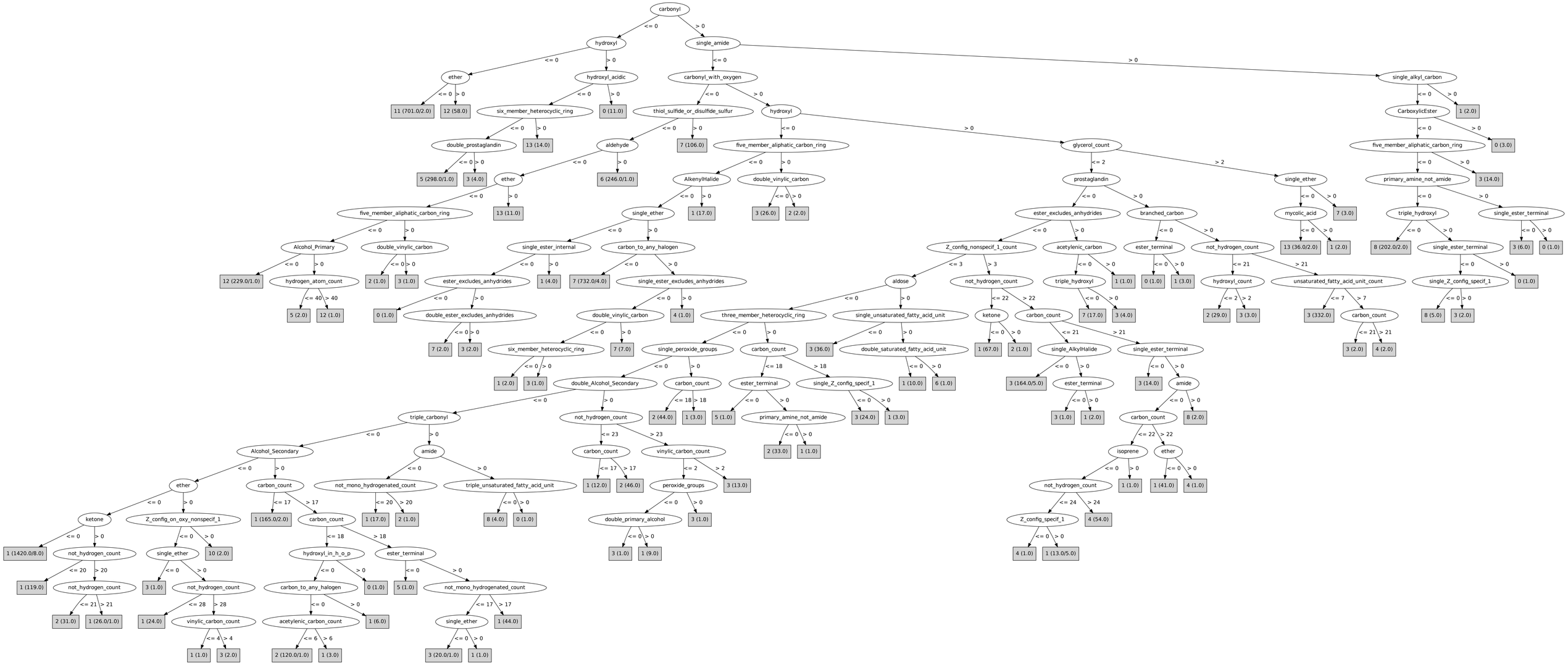
carbonyl
<= 0
> 0
hydroxyl
single_amide
ether
hydroxyl_acidic
carbonyl_with_oxygen
single_alkyl_carbon
11 (701.0/2.0)
12 (58.0)
six_member_heterocyclic_ring
0 (11.0)
thiol_sulfide_or_disulfide_sulfur
CarboxylicEster
1 (2.0)
double_prostaglandin
13 (14.0)
aldehyde
7 (106.0)
five_member_aliphatic_carbon_ring
glycerol_count
0 (3.0)
5 (298.0/1.0)
3 (4.0)
6 (246.0/1.0)
AlkenylHalide
double_vinylic_carbon
prostaglandin
single_ether
primary_amine_not_amide
3 (14.0)
13 (11.0)
1 (17.0)
3 (26.0)
2 (2.0)
ester_excludes_anhydrides
branched_carbon
mycolic_acid
7 (3.0)
triple_hydroxyl
single_ester_terminal
Alcohol_Primary
single_ester_internal
carbon_to_any_halogen
Z_config_nonspecif_1_count
acetylenic_carbon
ester_terminal
not_hydrogen_count
13 (36.0/2.0)
1 (2.0)
8 (202.0/2.0)
3 (6.0)
0 (1.0)
12 (229.0/1.0)
hydrogen_atom_count
2 (1.0)
3 (1.0)
1 (4.0)
7 (732.0/4.0)
single_ester_excludes_anhydrides
aldose
1 (1.0)
0 (1.0)
1 (3.0)
hydroxyl_count
unsaturated_fatty_acid_unit_count
single_Z_config_specif_1
5 (2.0)
12 (1.0)
0 (1.0)
double_ester_excludes_anhydrides
double_vinylic_carbon
4 (1.0)
three_member_heterocyclic_ring
single_unsaturated_fatty_acid_unit
ketone
carbon_count
2 (29.0)
3 (3.0)
3 (332.0)
8 (5.0)
3 (2.0)
7 (2.0)
3 (2.0)
7 (7.0)
3 (36.0)
double_saturated_fatty_acid_unit
1 (67.0)
2 (1.0)
7 (17.0)
3 (4.0)
single_AlkylHalide
3 (2.0)
4 (2.0)
six_member_heterocyclic_ring
single_peroxide_groups
1 (2.0)
3 (1.0)
double_Alcohol_Secondary
1 (10.0)
6 (1.0)
3 (164.0/5.0)
3 (14.0)
amide
triple_carbonyl
not_hydrogen_count
3 (24.0)
1 (3.0)
3 (1.0)
1 (2.0)
8 (2.0)
Alcohol_Secondary
vinylic_carbon_count
2 (33.0)
1 (1.0)
isoprene
ether
1 (12.0)
2 (46.0)
3 (13.0)
1 (1.0)
1 (41.0)
4 (1.0)
1 (165.0/2.0)
not_mono_hydrogenated_count
triple_unsaturated_fatty_acid_unit
peroxide_groups
1 (17.0)
2 (1.0)
8 (4.0)
0 (1.0)
double_primary_alcohol
3 (1.0)
4 (54.0)
1 (1420.0/8.0)
Z_config_on_oxy_nonspecif_1
hydroxyl_in_h_o_p
ester_terminal
3 (1.0)
1 (9.0)
Z_config_specif_1
10 (2.0)
1 (119.0)
3 (1.0)
carbon_to_any_halogen
0 (1.0)
5 (1.0)
not_mono_hydrogenated_count
4 (1.0)
1 (13.0/5.0)
2 (31.0)
1 (26.0/1.0)
1 (24.0)
vinylic_carbon_count
acetylenic_carbon_count
1 (6.0)
single_ether
1 (44.0)
1 (1.0)
3 (2.0)
2 (120.0/1.0)
1 (3.0)
3 (20.0/1.0)
1 (1.0)