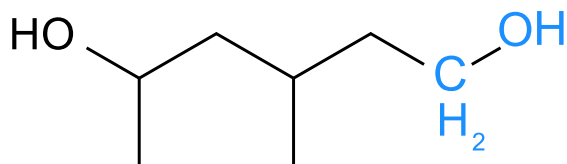
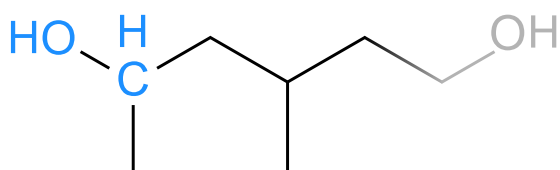


Example 2: pure aliphatic alcohol/polyol compound:  
SMILES CC(O)CC(C)CCO

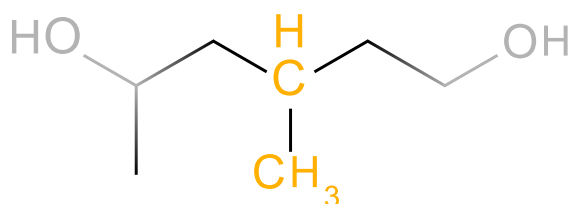
- 1 **Step 1:** detect hydroxyl groups and the  $\text{CH}_n$  groups directly bonded to them;  
SMARTS [CH2][OX2H1]  
1 match: ALOMFAC subgroup 150, ( $\text{CH}_2^{[\text{OH}]}$ ), alkyl bonded to OH  
and subgroup 153, (OH), hydroxyl



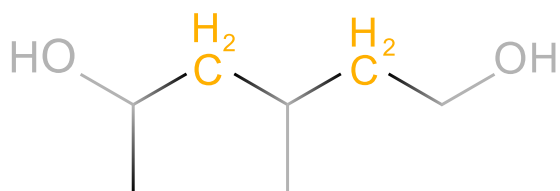
- 2 SMARTS [CH1][OX2H1]  
1 match: ALOMFAC subgroup 151, ( $\text{CH}^{[\text{OH}]}$ ), alkyl bonded to hydroxyl group  
and subgroup 153, (OH), hydroxyl



- 3 **Step 2a:** determine end groups of hydrophobic tail chains terminating in  $-\text{CH}_n-\text{CH}_3$ ;  
SMARTS [CH3][CH1]  
1 match: ALOMFAC subgroup 145, ( $\text{CH}_3^{[\text{alc-tail}]}$ ), alkyl in hydrophobic tail  
and subgroup 147, ( $\text{CH}^{[\text{alc-tail}]}$ ), alkyl in hydrophobic tail



- 4 **Step 2b:** determine all  $-\text{CH}_n-$  groups within hydrophobic tail chains;  
SMARTS [CX4], additional condition: must be neighbor of another hydrophobic tail group;  
2 matches: ALOMFAC subgroup 146, ( $\text{CH}_2^{[\text{alc-tail}]}$ ), alkyl in hydrophobic tail



- 5 **Step 3:** assign "alkyl within alcohols" type to all remaining  $-\text{CH}_n-$  groups.  
SMARTS [CH3]  
1 match: ALOMFAC subgroup no. 141, ( $\text{CH}_2^{[\text{alc}]}$ ), alkyl in alcohols

