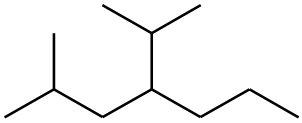
2

The language of organic chemistry

Answers to worked examples

WE 2.1 Naming alkanes (p. 83)

Give the IUPAC name of the following compound.

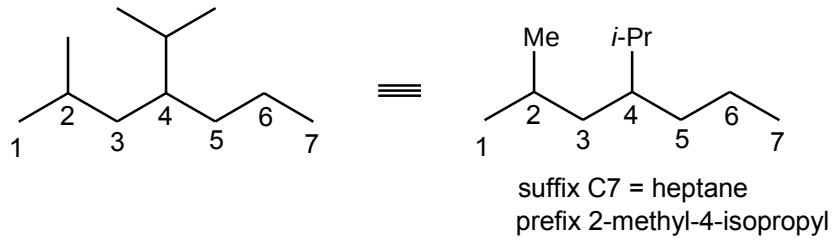


Strategy

1. Use the rules on p.82.
2. Identify the longest continuous carbon chain. All alkane names end with –ane.
3. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
4. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has SEVEN carbon atoms; and therefore its suffix is heptane.
2. For this molecule, the carbon atoms are numbered from left to right as 4-isopropyl-2-methyl has lower numbers than 4-isopropyl-6-methyl. [Remember: **i**sopropyl comes before **m**ethyl, as **i** is before **m** in the alphabet.]
3. The name of this compound is 4-isopropyl-2-methylheptane.



Answer

4-Isopropyl-2-methylheptane

WE 2.2 Skeletal structures and classifying carbon atoms (on p. 84)

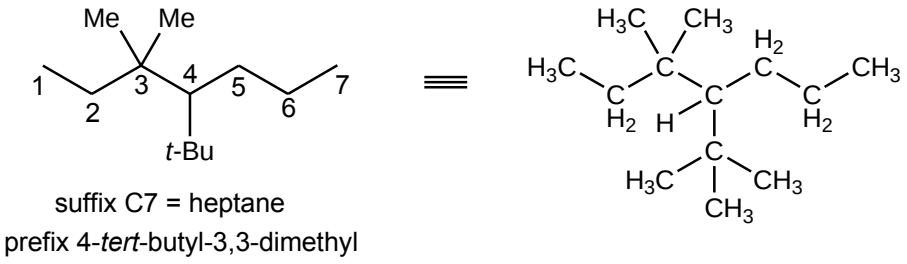
Draw the skeletal structure of 4-*tert*-butyl-3,3-dimethylheptane and label each of the carbon atoms as primary, secondary, tertiary, or quaternary.

Strategy

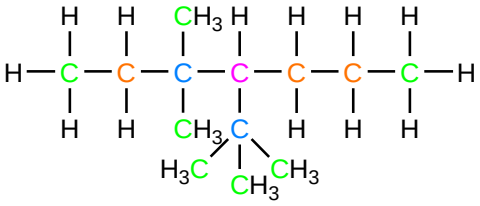
1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct!
4. To determine whether each carbon atom is primary, secondary, tertiary or quaternary, count the number of carbon atoms attached to it.

Solution

1. This molecule is an alkane. The longest number of continuous carbon atoms is seven (**hept**ane). Draw out this carbon chain.
2. There are two different substituents; a *tert*-butyl (Me_3C-) group at carbon-4, and two methyl (Me-) groups at carbon-3.
3. Name the structure that has been drawn (just to double check). This structure is 4-*tert*-butyl-3,3-dimethylheptane.



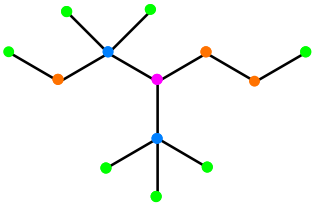
4. Primary (1^o), secondary (2^o), tertiary (3^o) and quaternary (4^o) carbon atoms are bonded to one, two, three and four carbon atoms, respectively.



C = primary carbon
C = secondary carbon
C = tertiary carbon atom
C = quaternary carbon atom

4-*tert*-butyl-3,3-dimethylheptane

Answer



Green = primary carbon
Orange = secondary carbon
Purple = tertiary carbon
Blue = quaternary carbon

4-*tert*-butyl-3,3-dimethylheptane

WE 2.3 Naming alkenes (on p. 87)

Draw the *cis*-, *cis*- and *cis*-, *trans*- isomers of octa-3,5-diene.

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Draw out the double bonds at their designated positions.
3. A *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond. A diene contains two C=C bonds.
4. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
5. Check that this structure is correct!

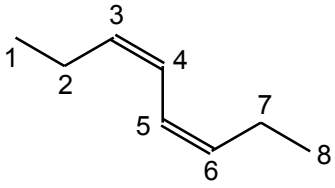
Solution

1. The longest number of continuous carbon atoms is eight (**octa**-3,5-diene). Draw out this carbon chain for both isomers.

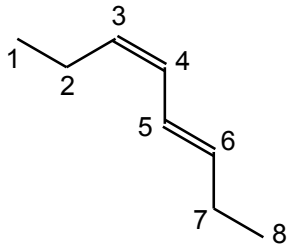
2. The suffix of this molecule is ene (octa-3,5-di**ene**); it is therefore an alkene. This molecule contains two double bonds (octa-3,5-**di**ene), and they are positioned at carbons **3** (→4) and **5** (→6).

suffix C8 = **octa**-3,5-di**ene**

3. The *cis*, *cis*-isomer is where both double bonds at carbons **3** (→4) and **5** (→6) have their substituents on the *same side* of the double bond. For the stereoisomeric *cis*-, *trans*-isomer, the double bonds at carbons **3** (→4) and **5** (→6) have *cis*- and *trans*-configurations, respectively. A *trans*-isomer is where the substituents are on *opposite sides* of the double bond. A diene contains two C=C bonds.



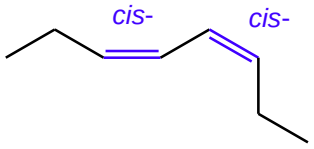
cis-,*cis*-octa-3,5-diene



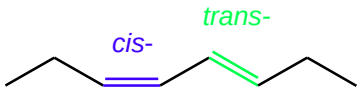
cis-,*trans*-octa-3,5-diene

4. There are no additional substituents.
5. Check that these structures are correct by re-naming it! This structure is 4-*tert*-butyl-3,3-dimethylheptane.

Answer



cis-,*cis*-octa-3,5-diene



cis-,*trans*-octa-3,5-diene

WE 2.4 Naming substituted benzenes (on p. 89)

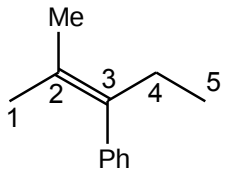
Draw the skeletal structure of 2-methyl-3-phenylpent-2-ene.

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Draw out the double bond at its designated positions.
3. If stereochemistry is present; a *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.
4. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
5. Check that this structure is correct!

Solution

1. The longest number of continuous carbon atoms is five (**pent**-2-ene). Draw out this carbon chain.
2. The suffix of this molecule is ene (pent-2-**ene**); it is therefore an alkene. This molecule contains a single double bond (pent-2-**ene**), and this is positioned at carbons **2** to **3** (2→3).
3. There is no stereochemistry present.
4. There are two different substituents; a methyl (Me-) group at carbon-2, and a phenyl (Ph-) group at carbon-3.

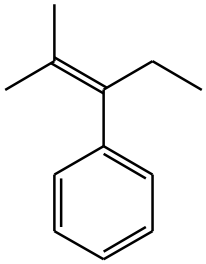


suffix C5 = **pent**-2-**ene**

prefix **2**-methyl-**3**-phenyl

5. Check that this structure is correct by re-naming it! This structure is 2-methyl-3-phenylpent-2-ene.

Answer



2-methyl-3-phenylpent-2-ene

WE 2.5 Naming halogenoalkenes (on p. 91)

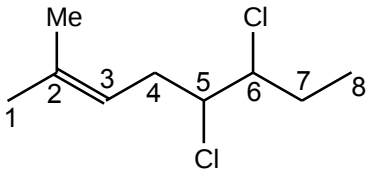
Draw the skeletal structure of 5,6-dichloro-2-methyloct-2-ene. Are the chlorine atoms bonded to primary, secondary, or tertiary carbon atoms?

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Draw out the double bond at its designated position.
3. If stereochemistry is present; a *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.
4. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
5. Check that this structure is correct!

Solution

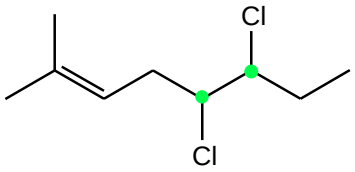
1. The longest number of continuous carbon atoms is eight (**oct**-2-ene). Draw out this carbon chain.
2. The suffix of this molecule is ene (oct-2-**ene**); it is therefore an alkene. This molecule contains a single double bond (oct-2-**ene**), and this is positioned at carbons **2** to **3** (2→3).
3. There is no stereochemistry present.
4. There are two different substituents; a methyl (Me-) group at carbon-2, and two chloro-substituents at carbons-5 and 6.



suffix C8 = **oct**-2-**ene**
prefix **5**,**6**-dichloro-**2**-methyl

5. Check that this structure is correct by re-naming it! This structure is 5,6-dichloro-2-methyloct-2-ene.

Answer



● = secondary carbon atom
5,6-dichloro-2-methyloct-2-ene

WE 2.6 Naming and classifying alcohols (on p. 93)

Draw the skeletal structure of 1-methyl-2-vinylcyclopentanol. Is this a primary, secondary, or tertiary alcohol?

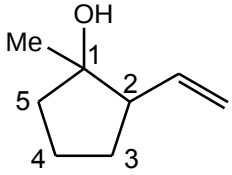
Strategy

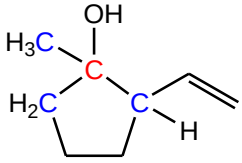
1. Draw out the skeleton structure of cyclopentane and remember to number the carbon atoms.
2. Identify the substituents from their prefix, and place them along this carbon chain at their designated positions. As this molecule is cyclopentanol, the OH group is at position 1.
3. Check that the structure you have drawn is correct!
4. Count the number of alkyl groups attached to the carbon atom bearing the OH group to determine if this alcohol is primary (1^o), secondary (2^o) or tertiary (3^o).

Solution

1. Cyclopentane is a cyclic ring of five carbon atoms (cyclo**pent**anol). Draw out this cycloalkane. The suffix of this molecule is -ol (cyclopentan**ol**); it is therefore an alcohol.

2. As this molecule is cyclopentanol, the OH group is at position 1. There are two additional substituents; a methyl (Me-) group at carbon-1, and a vinyl (CH_2=CH-) group at carbon-2.



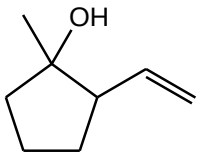


suffix C5 = cyclo**pent**anol
prefix **1**-methyl-**2**-vinyl

a tertiary alcohol

3. This alcohol is a tertiary alcohol as the (red) carbon bearing the OH group has THREE (blue) alkyl groups attached to it.

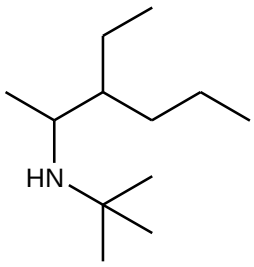
Answer



1-methyl-2-vinylcyclopentanol
(a tertiary alcohol)

WE 2.7 Naming and classifying amines (on p. 96)

Give the IUPAC name of the following amine and classify the amine as primary, secondary, or tertiary.



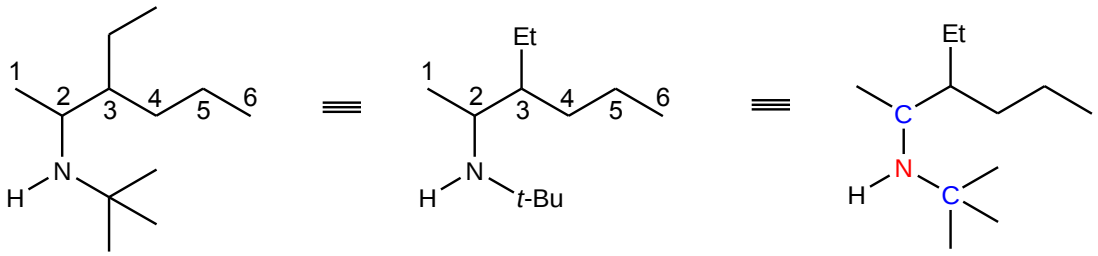
Strategy

1. Identify the longest continuous carbon chain and remember to number the carbon atoms so that the amine group has the lowest possible number.
2. Identify the two remaining groups attached to the nitrogen atom of this amine; this name is preceded by *N*,*N*- (which states that these substituents are attached to this nitrogen atom).

3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.
4. Count the number of alkyl groups attached to this nitrogen atom to determine if this amine is primary (1^o), secondary (2^o) or tertiary (3^o).

Solution

1. The longest continuous carbon chain has SIX carbon atoms; and therefore its suffix is **hex**ane. For this alkanamine, the (lowest possible number for this) amine group is on carbon-2.
2. The two remaining groups attached to this nitrogen atom are *tert*-butyl and hydrogen. This amine is *N*-*tert*-butyl amine.
3. There is one remaining substituent, an ethyl (Et) group at carbon-3. This amine is 3-ethylhexan-2-amine. Its overall name is *N*-*tert*-butyl-3-ethylhexan-2-amine.



suffix C6 = hexan-2-amine | prefix *N*-*tert*-butyl-**3**-ethyl | a secondary amine

4. This amine is a secondary amine as the (red) nitrogen atom has TWO (blue) alkyl groups attached to it. The name of this compound is *N*-*tert*-butyl-3-ethylhexan-2-amine.

Answer

N-*tert*-butyl-3-ethylhexan-2-amine. This is a secondary amine.

WE 2.8 Naming ketones (on p. 100)

Draw the skeletal structure of 2-allyl-3,3-dimethylhexanal.

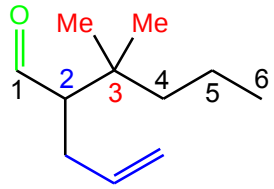
Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.

2. Identify the substituents from their prefix, and place them along this carbon chain at their designated positions.
3. Check that the structure you have drawn is correct!

Solution

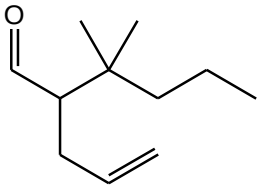
1. The longest number of continuous carbon atoms is six (**hexan**ol). Draw out this carbon chain. This molecule is an aldehyde (hexan**al**); the aldehyde group is at carbon-1.
2. There are two different substituents; an allyl group (CH_2=CH-CH_2-) at carbon-2, and two methyl (Me-) groups at carbon-3.



suffix C6 = **hex**anal
prefix 2-allyl-3,3-dimethyl

3. Check that this structure is correct by re-naming it! This structure is 2-allyl-3,3-dimethylhexanal.

Answer



2-allyl-3,3-dimethylhexanal

WE 2.9 Drawing and naming esters (on p. 103)

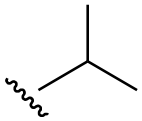
Draw the skeletal structure of isopropyl benzoate.

Strategy

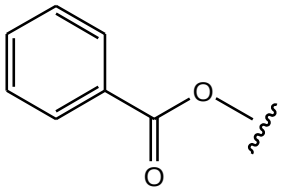
1. This molecule is an isopropyl ester. The parent carboxylate is benzoate. Draw out the carbon skeleton of these components.
2. Check that the structure you have drawn is correct!

Solution

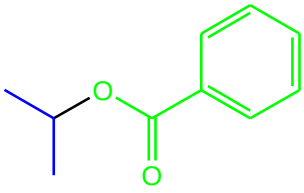
1. An isopropyl group is Me_2CH-, and a benzoate group is $PhCO_2$-. By connecting these two fragments together reveals the structure of the required ester.



an isopropyl group



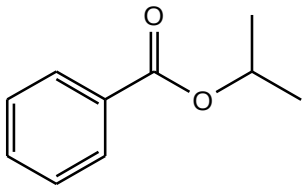
a benzoate group



isopropyl benzoate

2. Check that this structure is correct by re-naming it! This structure is isopropyl benzoate.

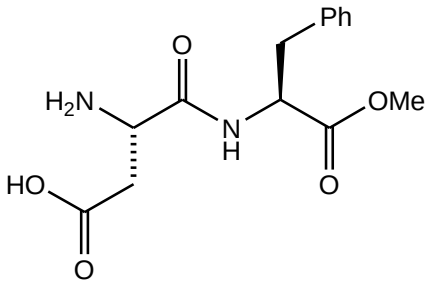
Answer



isopropyl benzoate

WE 2.10 Spotting functional groups (on p. 105)

Name all five functional groups in aspartame.



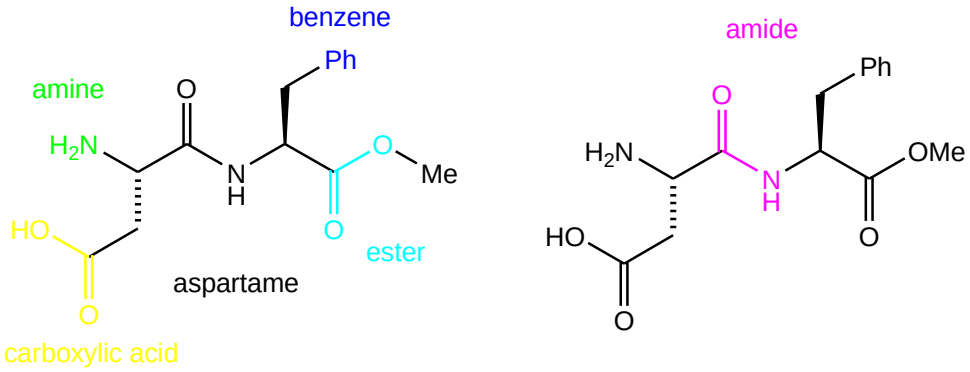
Strategy

1. Carefully consider the functionality of this molecule. It is important to note that the alkane backbone of this molecule is not a functional group but a carbon skeleton.

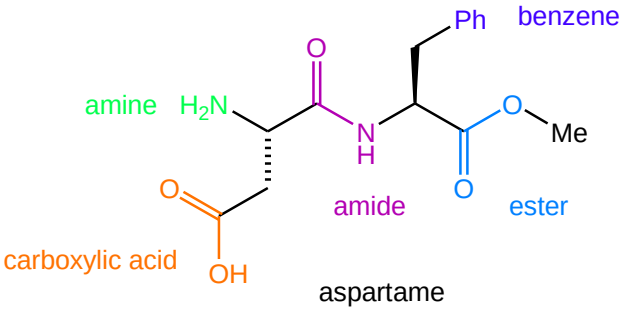
Solution

1. This molecule contains five functional groups. There are three obvious functional groups; the carboxylic acid (RCO_2H), the primary amine ($-NH_2$) and the ester ($R^1CO_2R^2$). The less obvious function group is the secondary amide (RC=ONHR); it

should not be confused as two separate functional groups, namely a ketone (C=O) and a secondary amine (-NHR). The remaining functional group is the phenyl (Ph-) ring; this is classed a benzene functional group.



Answer



Answers to boxes

Box 2.5 The DDT dilemma (on p. 91)

Some insects have developed a resistance to DDT by producing enzymes that catalyse the conversion of DDT into a related compound called 1,1-dichloro-2,2-di(4-chlorophenyl)ethene (DDE). DDE is not an insecticide as this compound is flatter than DDT and the change in shape alters the toxicity.

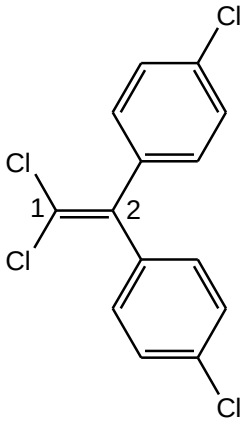
Draw the skeletal structure for DDE.

Strategy

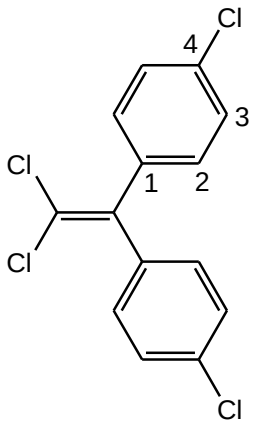
1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Draw out the double bond at its designated positions.
3. If stereochemistry is present; a *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.
4. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
5. Check that this structure is correct!

Solution

1. The longest number of continuous carbon atoms is two (**eth**ene). Draw out this carbon chain.
2. The suffix of this molecule is ene (eth**ene**); it is therefore an alkene. This molecule contains a single double bond, and this is positioned at carbon **1** (→2).
3. There is no stereochemistry present.
4. There are two different substituents; two chloro- (Cl-) substituents at carbon-1, and two 4-chlorophenyl- (4-ClC_6H_4-) groups at carbon-2.



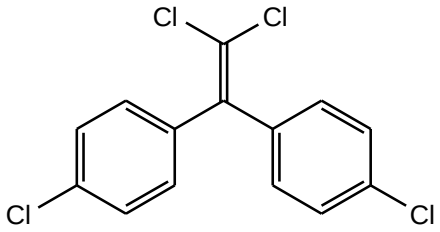
suffix C2 = ethene



prefix 1,1-dichloro-2,2-di(4-chlorophenyl)

5. Check that this structure is correct by naming it! This structure is 1,1-dichloro-2,2-di(4-chlorophenyl)ethene.

Answer



1,1-dichloro-2,2-di(4-chlorophenyl)ethene

Answers to end of chapter questions (on p. 109)

1. Draw skeletal structures of the following compounds:

(a) 2,3,5-trimethylhexane

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct!

Solution

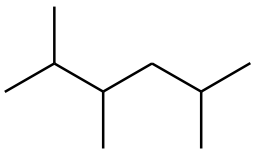
1. This molecule is an alkane. The longest number of continuous carbon atoms is six (**hex**ane). Draw out this carbon chain.
2. There are three methyl (Me) groups at carbons-2, -3 and -5.

suffix C6 = hexane prefix 2,3,5-trimethyl

3. Name the structure that you have drawn (just to double check). This structure is 2,3,5-trimethylhexane.

Answer

This structure is 2,3,5-trimethylhexane.



2,3,5-trimethylhexane

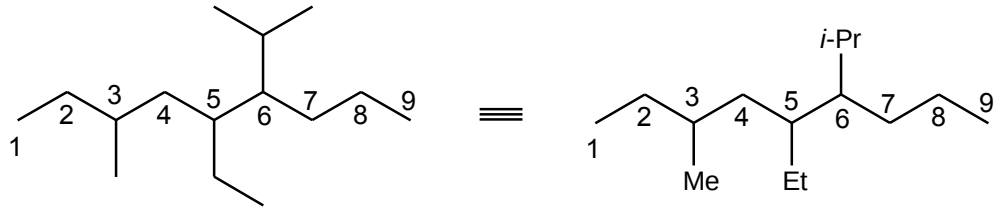
(b) 5-ethyl-6-isopropyl-3-methylnonane.

Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct!

Solution

1. This molecule is an alkane. The longest number of continuous carbon atoms is nine (**non**ane). Draw out this carbon chain.
2. There are three substituents, a methyl (Me) group at carbon-3, an ethyl (Et) at carbon-5, and an isopropyl (*i*-Pr) group at carbon-6.

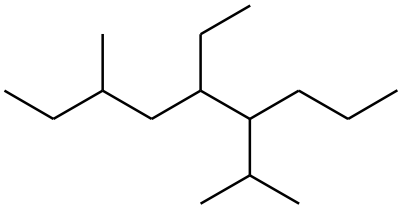


suffix C9 = nonane prefix 5-ethyl-6-isopropyl-3-methyl

3. Name the structure that you have drawn (just to double check). This structure is 2,3,5-trimethylhexane.

Answer

This structure is 2,3,5-trimethylhexane.



5-ethyl-6-isopropyl-3-methylnonane

2. Draw skeletal structures and give the names of the five structural isomers of a hydrocarbon with a molecular formula C_6H_{14}.

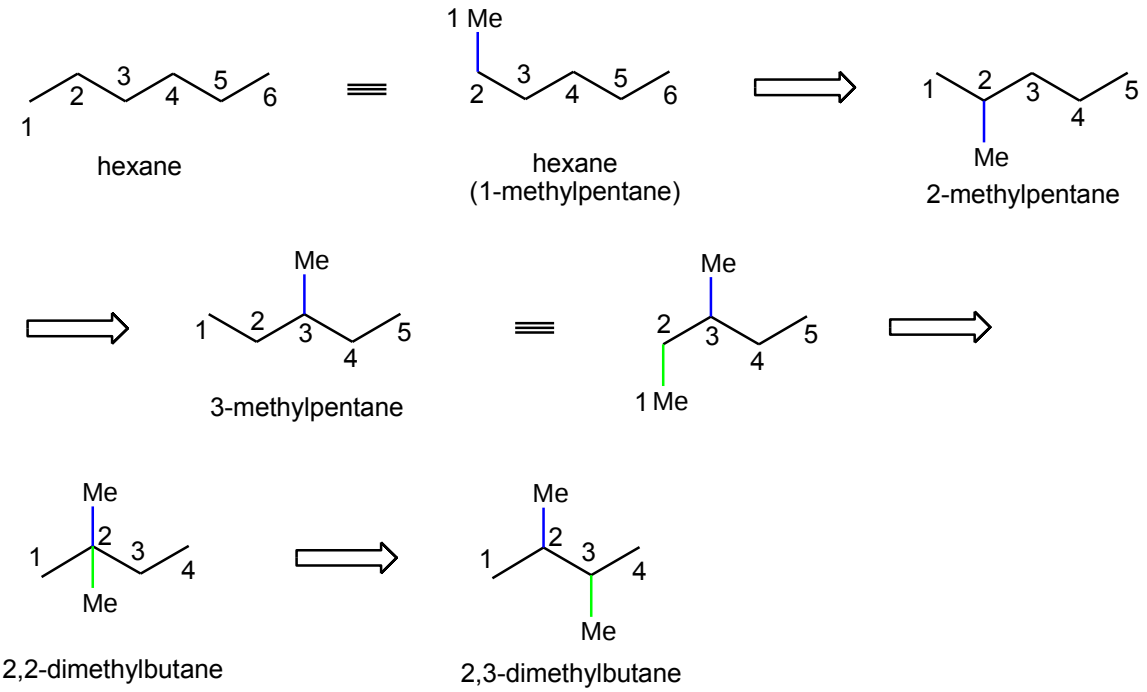
Strategy

From this formula, C_6H_{14}, hexane is the simplest structural isomer as it is consists of a straight chain of six-carbon atoms in a *zig-zag* arrangement.

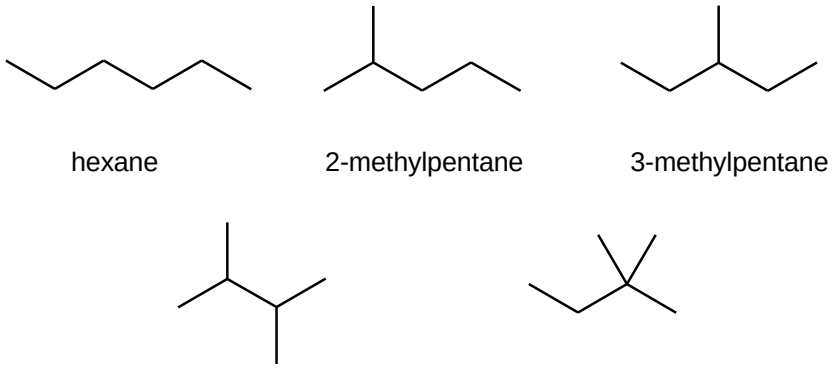
In order to draw the remaining structural isomers, a branching methyl group will need to be introduced at carbon-2 to give 2-methylpentane. [This can be thought of as moving the methyl group from carbon-1 of "1-methylpentane" (hexane) to carbon-2 to give 2-methylpentane.] This process can be re-iterated once more to give 3-methylpentane. However, it can be repeated again to give "4-methylpentane"; this molecule is the same as 2-methypentane.

The next generation of structural isomers can be drawn by repeating this process on either 2-methylpentane or 3-methylpentane to give 2,3-dimethylbutane and 2,2-dimethylbutane.

Solution



Answer



hexane 2-methylpentane 3-methylpentane

2,3-dimethylbutane 2,2-dimethylbutane

3. Draw skeletal structures of the following compounds:

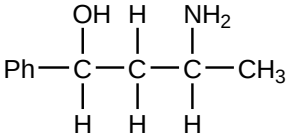
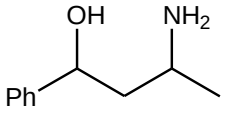
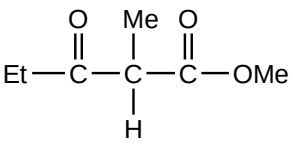
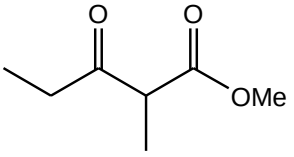
(a) $PhCH(OH)CH_2CH(NH_2)CH_3$;

(b) $EtCOCH(Me)CO_2Me$;

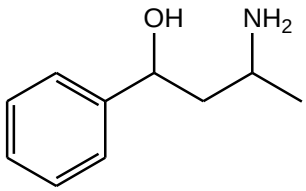
Strategy

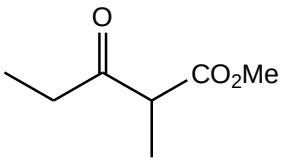
In order to draw out these molecules as skeletal structures, their full structural formula must first be drawn. These can be easily converted into skeletal structures by omitting the hydrogen atoms attached to carbon atoms. Invariably, skeletal structures are drawn in a *zig-zag* arrangement involving the longest carbon chain.

Solution

	Full structural formulae	Condensed structures	Skeletal structures
(a)	$PhCH(OH)CH_2CH(NH_2)CH_3$		
(b)	$EtCOCH(Me)CO_2Me$		

Answers

(a) 

(b) 

(c) $Me_2C{=}CHCH_2CH_2C(CH_3){=}CHCH_2OH$;

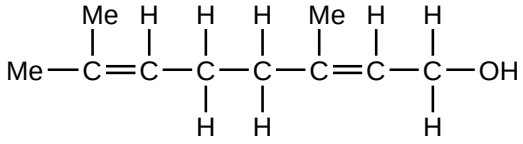
Strategy

In order to draw out this molecule as a skeletal structure, the full structural formula must first be drawn. This can be easily converted into a skeletal structure by omitting the hydrogen atoms attached to carbon atoms. Invariably, skeletal structures are drawn in a *zig-zag* arrangement involving the longest carbon chain. For molecules that contain alkene functionality, there may be stereoisomerism to consider.

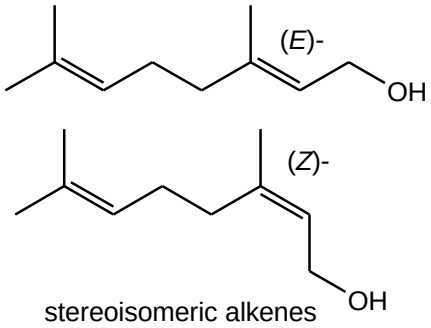
Solution

For this molecule, only one of its two double bonds can be stereoisomeric. These are labelled as (*E*)- and (*Z*)- in accordance with the Cahn-Ingold-Prelog rules (see p. 839).

Full structural formula $Me_2C{=}CHCH_2CH_2C(CH_3){=}CHCH_2OH$

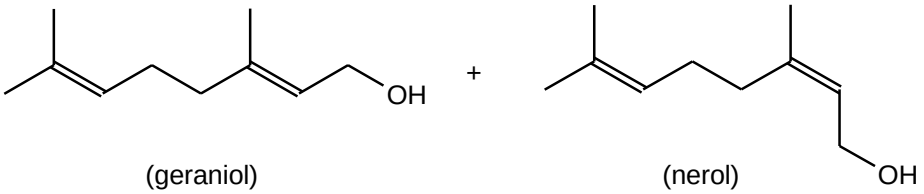
Condensed structure 

Skeletal structures



stereoisomeric alkenes

Answer



(geraniol) (nerol)

(d) 5-(3-nitrophenyl)-5-oxopentanoic acid.

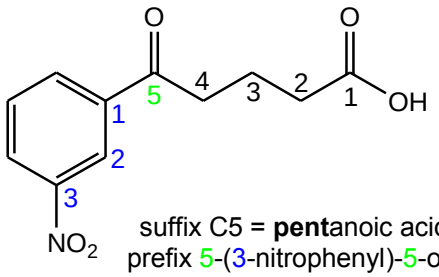
Strategy

1. Draw out the longest continuous carbon chain as a *zig-zag* structure and remember to number the carbon atoms.
2. Identify the substituents from their suffix, and place them along this carbon chain at their designated positions.
3. Check that this structure is correct by re-naming it!
4. Re-draw, if necessary, into the required skeletal structure.

Solution

1. The longest number of continuous carbon atoms is five (**pent**anoic acid). Draw out this carbon chain. The suffix of this molecule is -oic (pentan**oic** acid); it is therefore a carboxylic acid. The carboxylic acid group is at carbon-1.
2. There are two different substituents at carbon-5; a 3-nitrophenyl group and an oxo- (=O) group (commonly known as a carbonyl group).

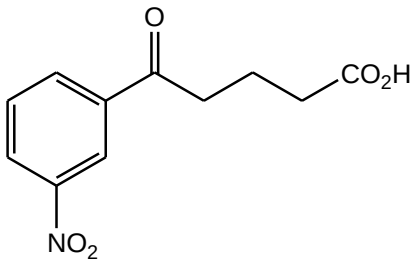
5-(3-nitrophenyl)-5-oxopentanoic acid



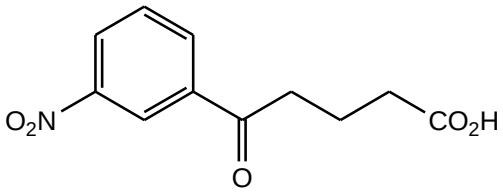
suffix C5 = **pent**anoic acid
prefix 5-(3-nitrophenyl)-5-oxo

3. This structure is this correct. It is 5-(3-nitrophenyl)-5-oxopentanoic acid.

4. The skeletal structure is:

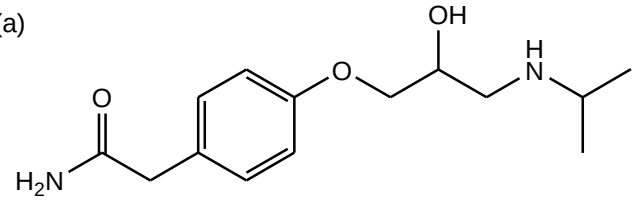


Answer



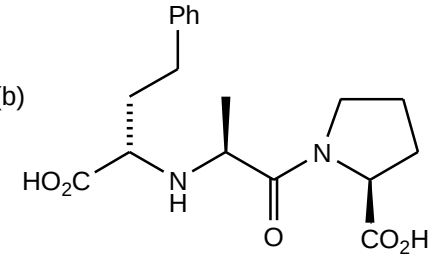
4. Name all of the functional groups in the following molecules.

(a)



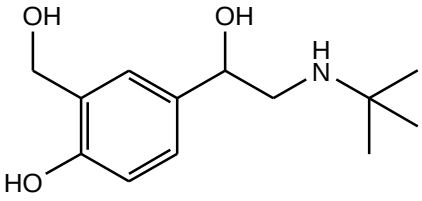
atenolol
Used for the treatment and
prevention of heart disease

(b)



enalaprilat
Used for the treatment of
high blood pressure (hypertension)

(c)



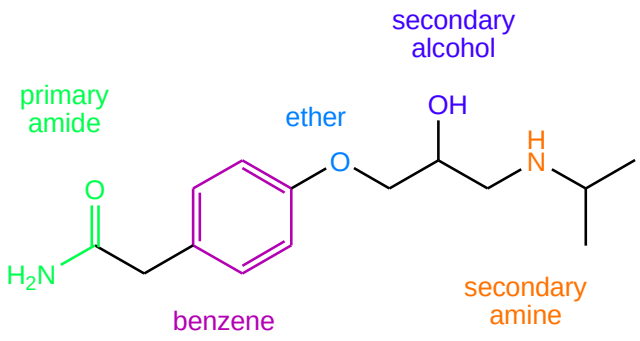
salbutamol
Used for the treatment of asthma

Strategy

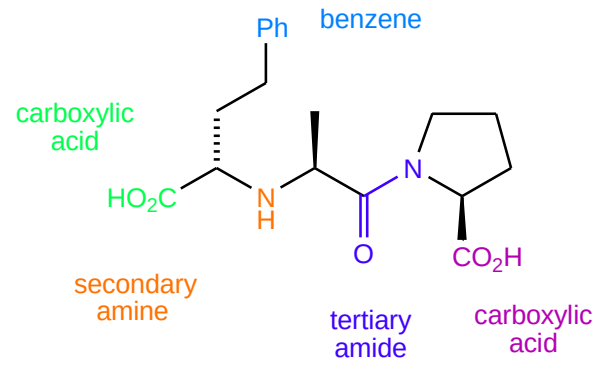
Carefully consider the functionality of each molecule. It is important to note that the alkane backbone of these molecules is not a functional group but a carbon skeleton. A functional group is a group which is able to change its function using a suitable reaction.

Solution

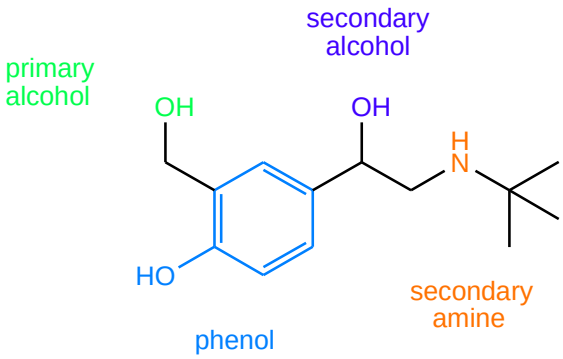
(a)



(b)



(c)



Answers

(a) Atenolol contains FIVE functional groups; primary amide, benzene, ether, secondary alcohol and secondary amine.

(b) Enalaprilat contains FOUR different functional groups; secondary amine, benzene, tertiary amide and two carboxylic acids.

(c) Salbutamol contains FOUR functional groups; primary alcohol, secondary alcohol, phenol and secondary amine.

5. Give IUPAC names for the following compounds:

(a) $BrCH_2CH_2CH_2CHMe_2$

Strategy

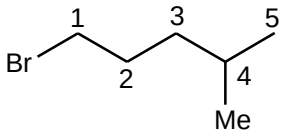
1. Identify the longest continuous carbon chain. All alkane names end with –ane.
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).

3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has **FIVE** carbon atoms; therefore its suffix is **pent**ane.
2. For this molecule, the carbon atoms are numbered from left to right as 1-bromo-4-methyl- has lower numbers than 2-methyl-5-bromo-. [Remember **b**romo comes before **m**ethyl as **b** comes before **m** in the alphabet.]

$BrCH_2CH_2CH_2CHMe_2$



suffix C5 = **pent**ane
prefix 1-bromo-4-methyl

3. The name of this compound is 1-bromo-4-methylpentane.

Answer

1-Bromo-4-methylpentane

(b) $H_2C{=}CHCH_2OH$

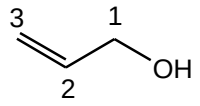
Strategy

1. Identify the longest continuous carbon chain. Draw out this chain. This molecule is an alcohol, so its suffix will be -ol (*c.f.* alcoh**ol**).
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has **THREE** carbon atoms; and as this molecule is an alcohol, its suffix is **propan**ol.
2. As this molecule is propanol, the -OH group is at position-1. The remaining functional group, alkene, is at carbon-2 (→3).

$H_2C{=}CHCH_2OH$



suffix C3 = **prop**anol
functional group = 2-ene

3. The name of this compound is prop-2-en-1-ol.

Answer

Prop-2-en-1-ol

(c) $H_2NCH_2CH_2CO_2Me$.

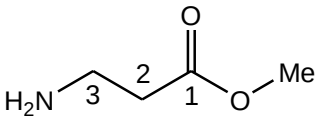
Strategy

1. Identify the longest continuous carbon chain. Draw out this chain. This molecule is an ester, so its suffix will be -oate.
2. Number the carbon atoms starting at the end nearest to a branch point (to ensure the substituents have the lowest possible numbers).
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The longest continuous carbon chain has **THREE** carbon atoms; and as this molecule is an ester, its suffix is **propan**oate.
2. This molecule is a **methyl** ester. The C=O group is at position-1. The remaining functional group, amine, is at carbon-3.

$H_2NCH_2CH_2CO_2Me$



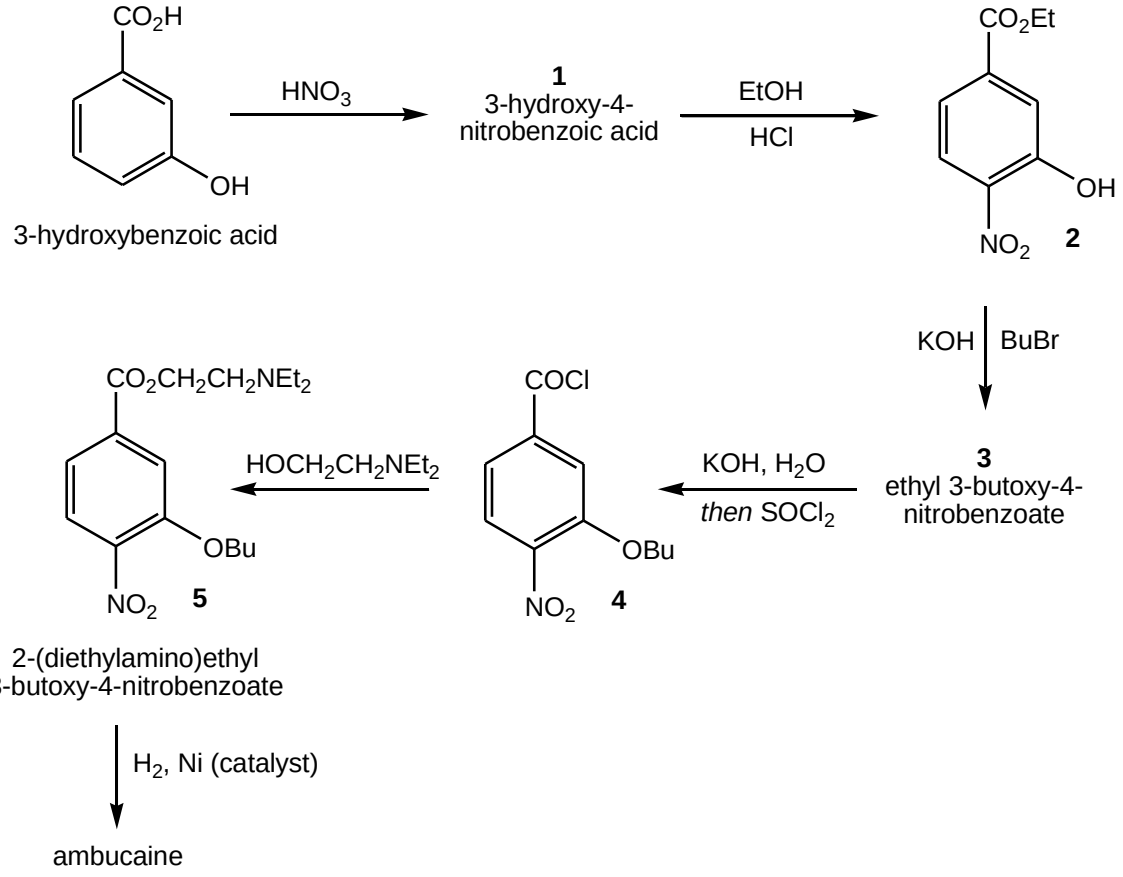
suffix C3 = **prop**anoate
prefix = 3-amino

3. The name of this compound is methyl-3-aminopropanoate.

Answer

Methyl-3-aminopropanoate

6. The following questions relate to the synthesis of the local anaesthetic ambucaine, starting from 3-hydroxybenzoic acid, which is shown in the scheme below.



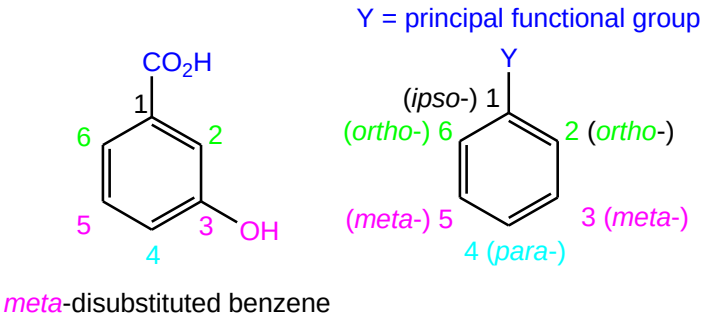
(a) Is 3-hydroxybenzoic acid an *ortho*-, *meta*- or *para*-disubstituted benzene?

Strategy

1. Draw out this disubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around this benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned.
3. Deduce whether this molecule is an *ortho*-, *meta*- or *para*-disubstituted benzene.

Solution

1. The principal functional group is the carboxylic acid group (-CO_2H).
2. The carbon atom bearing this carboxylic acid group is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of any substituent.
3. This molecule is a 1,3-disubstituted benzene; it is also a *meta*-disubstituted benzene.



meta-disubstituted benzene

Answer

3-Hydroxybenzoic acid is a *meta*-disubstituted benzene.

(b) Draw skeletal structures for compounds **1** and **3**.

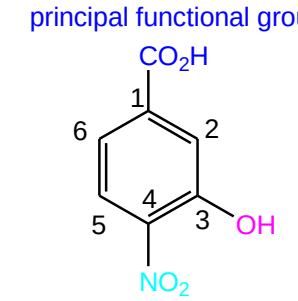
Compound **1** is 3-hydroxy-4-nitrobenzoic acid.

Strategy

1. Draw out this trisubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around this benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned.
3. Check that this structure is correct by re-naming it!

Solution

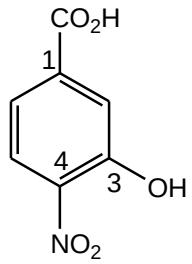
1. The principal functional group is the carboxylic acid group (-CO_2H).
2. The carbon atom bearing this carboxylic acid group is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of any substituents. The hydroxyl (-OH) group is on carbon-3, and the nitro (-NO_2) group is on carbon-4.



3-hydroxy-4-nitrobenzoic acid

3. This molecule is 3-hydroxy-4-nitrobenzoic acid. This reaction involves the introduction of a nitro (NO_2) group at carbon-4.

Answer



3-hydroxy-4-nitrobenzoic acid

Compound **3** is ethyl 3-butoxy-4-nitrobenzoate.

Strategy

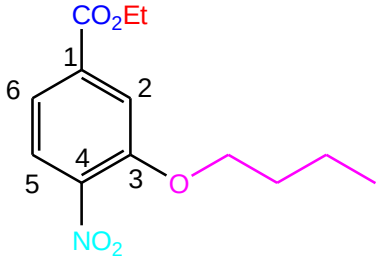
1. Draw out this trisubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around this benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned.
3. Check that this structure is correct by re-naming it!

Solution

1. The principal functional group is the carboxylate group (-**CO_2**-Et). This molecule is an ethyl ester (**ethyl** 3-butoxy-4-nitrobenz**oate**).
2. The carbon atom bearing this carboxylic acid group is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of

any substituents. A butoxy (-OBu) group is on carbon-3, and a nitro (-NO_2) is on carbon-4.

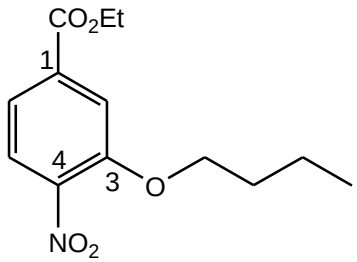
principal functional group



ethyl 3-butoxy-4-nitrobenzoic acid

3. This molecule is ethyl 3-butoxy-4-nitrobenzoic acid. This reaction involves the conversion of a hydroxyl (-OH) group into a butoxy (-OBu) group at carbon-3.

Answer



ethyl 3-butoxy-4-nitrobenzoic acid

(c) Give the IUPAC names for compounds **2** and **4**.

For compound 2:

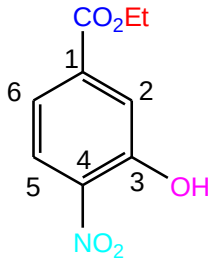
Strategy

1. Draw out this trisubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around this benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned and have the lowest possible numbers.
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The principal functional group is the carboxylate group (-**CO_2**-Et). This molecule is a substituted ethyl benzoate.
2. The carbon atom bearing this carboxylate ester group is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of any substituents. The hydroxy (-OH) group is on carbon-3, and the nitro (-NO_2) group is on carbon-4.

principal functional group



ethyl 3-hydroxy-4-nitrobenzoic acid

compound **2**

3. This molecule is ethyl 3-hydroxy-4-nitrobenzoate. [Note: these substituents are listed in alphabetical order.]

Answer

Ethyl 3-hydroxy-4-nitrobenzoate

For compound 4:

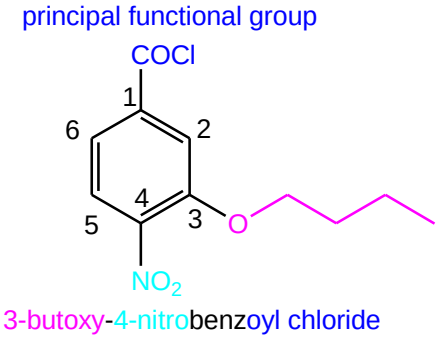
Strategy

1. Draw out this trisubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around this benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned and have the lowest possible numbers.
3. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The principal functional group is the acid chloride (-COCl). This molecule is a substituted benzoyl chloride.
2. The carbon atom bearing this acid chloride is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of any

substituents. The butoxy (-OBu) group is on carbon-3, and the nitro (-NO_2) group is on carbon-4.



3-butoxy-4-nitrobenzoyl chloride

compound **4**

3. This molecule is 3-butoxy-4-nitrobenzoyl chloride. [Note: these substituents are listed in alphabetical order.]

Answer

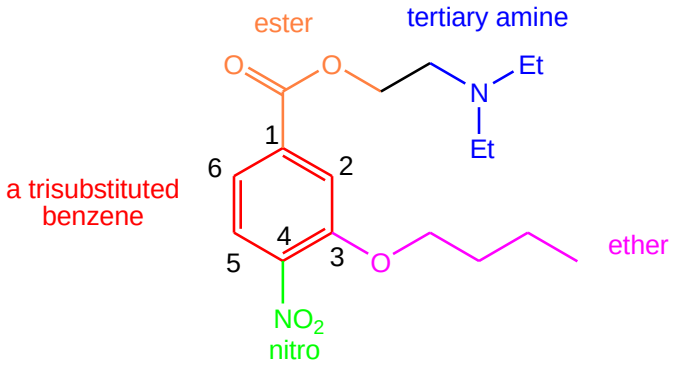
3-Butoxy-4-nitrobenzoyl chloride

(d) Name all the functional groups in compound **5**.

Strategy

This molecule contains five functional groups. There are four obvious functional groups, an ester group ($ArCO_2R$), a tertiary amine (-CH_2NEt_2), a nitro group (-NO_2) and an ether group (ArOR). The remaining functional group is the benzene ring itself.

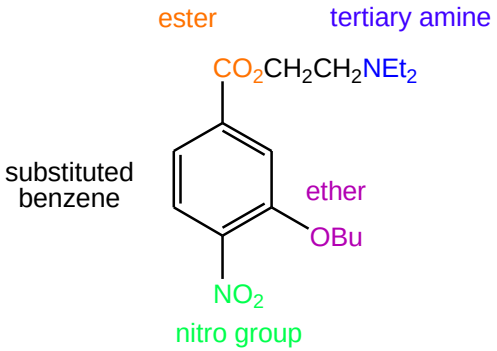
Solution



2-(diethylamino)ethyl 3-butoxy-4-nitrobenzoate

Compound **5**

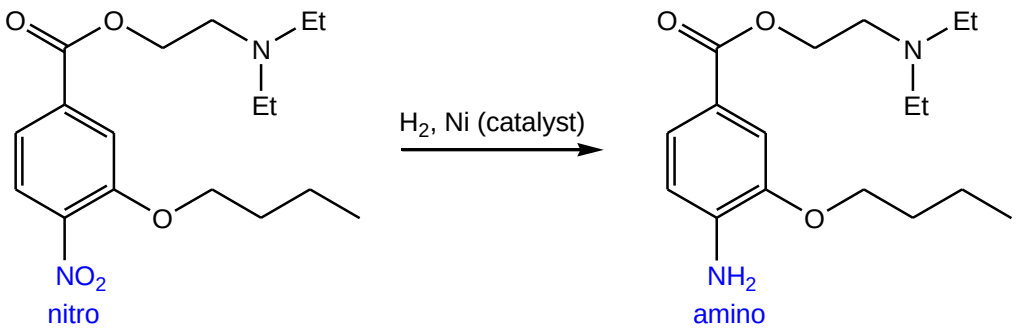
Answer



(e) Given that the $-NO_2$ group of compound **5** is reduced to an $-NH_2$ group, on reaction with H_2 and Ni (catalyst), draw a skeletal structure of ambucaine.

Strategy

Copy out the structure of compound **5**, and replace the nitro (NO_2-) group on carbon-4 with an amino ($-NH_2$) group to give the skeletal structure of ambucaine. The reaction scheme is shown below:



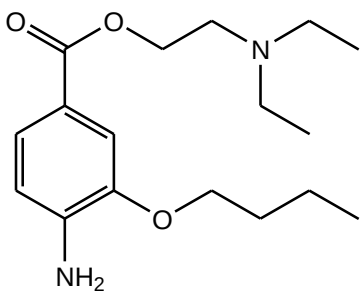
2-(diethylamino)ethyl 3-butoxy-4-nitrobenzoate

compound **5**

2-(diethylamino)ethyl 4-amino-3-butoxybenzoate

ambucaine

Answer



ambucaine

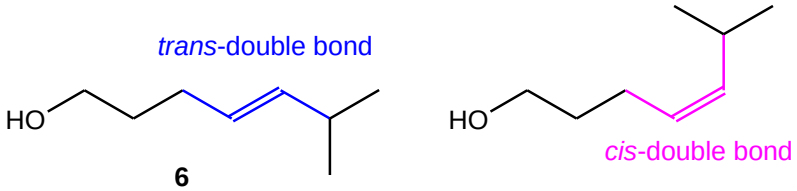
7. The hot spicy flavour of chilli peppers of the *Capsicum* family is due mainly to a compound called capsaicin. The following questions relate to the synthesis of capsaicin shown below.

(a) Draw a skeletal structure of the stereoisomer of alkene **6**.

Strategy

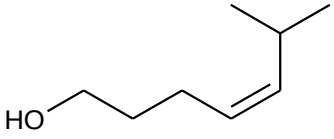
Molecule **6** is a di-substituted alkene and has *trans*-stereochemistry. The remaining stereoisomer of **6** must have *cis*-stereochemistry. [A *cis*-isomer is where both substituents are on the *same side* of the double bond, whereas, for a *trans*-isomer the substituents are on *opposite sides* of the double bond.]

Solution



6 stereoisomer of **6**

Answer



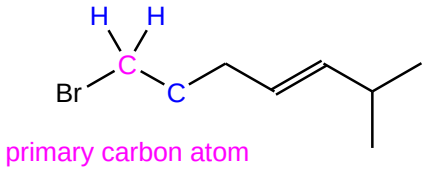
(b) In compound **7**, is the bromine bonded to a primary, secondary, or tertiary carbon atom?

Strategy

To determine whether this carbon atom bonded to the bromine atom is primary, secondary or tertiary, count the number of carbon atoms attached to it.

Solution

There is one carbon atom attached to the carbon atom bonded to the bromine atom. This carbon atom is primary.



primary carbon atom

7

Answer

The bromine atom is attached to a primary carbon atom.

(c) For the synthesis of compound **8**, $NaCH(CO_2Et)_2$ is prepared from $CH_2(CO_2Et)_2$, which has the common name diethyl malonate. Draw a skeletal structure of diethyl malonate and give the IUPAC name.

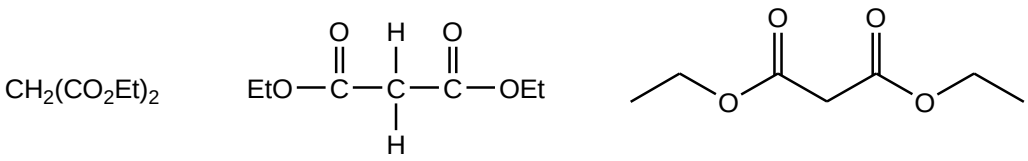
Strategy

In order to draw this molecule as a skeletal structure, the full structural formula must first be drawn out. This can be easily converted into its skeletal structure by omitting the hydrogen atoms attached to carbon atoms. Invariably, skeletal structures are drawn in a *zig-zag* arrangement involving the longest carbon chain.

To name this compound: identify the longest continuous carbon chain. Draw out this chain. This molecule contains two esters, so its suffix will be –**ate** and its prefix will be **di-**. Write down the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

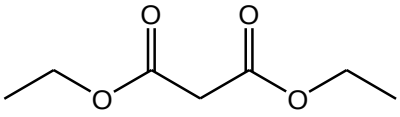
Full structural formula | Condensed structure | Skeletal structure



The longest continuous carbon chain has **THREE** carbon atoms; and as this molecule is a diester, its suffix will be **propane**dioate. This molecule is a **diethyl** ester.

The full IUPAC name of this molecule is diethyl propanedioate. Interesting, it could have also been called diethyl propane-1,3-dioate, but as there is no ambiguity of where these diesters are located, the locant "-1,3-" is not required.

Answer



diethyl propanedioate

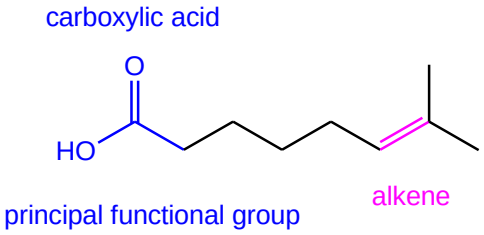
(d) Draw the structure of compound **8**, and indicate the α- and β-carbon atoms.

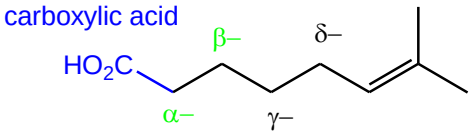
Strategy

The carbon atoms of a given molecule can be labelled sequentially away from its principle functional group; usually these carbon atoms are labelled using the Greek alphabet [*e.g.*, alpha- (α-), beta- (β -), gamma (γ-), delta (δ-) and so on ...].

Solution

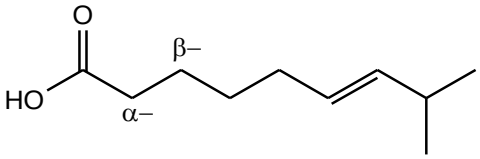
Molecule **8** contains two functional groups; the carboxylic acid is the principal functional group and the alkene is the secondary functional group; the α-carbon atom is adjacent to the principal functional group, and so on.



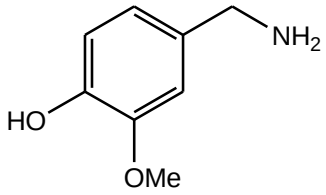


8

Answer



(e) Give the IUPAC name for compound **10.**



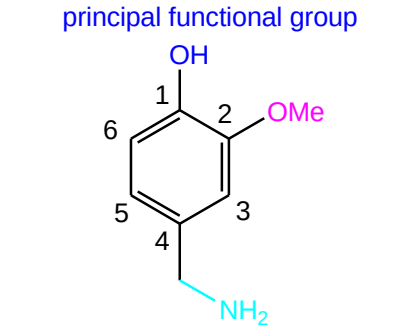
10

Strategy

1. Draw out this trisubstituted benzene, and identify its principal functional group.
2. Number the carbon atoms around the benzene ring, starting at its principal functional group. Ensure that any substituents are correctly positioned and have the lowest possible numbers.
3. Write out the complete name, and ensure that any substituents listed are in alphabetical order.

Solution

1. The principal functional group is the phenol group (ArOH).
2. The carbon atom bearing this phenolic (OH) group is carbon-1. Number the remaining carbons in a clockwise manner to ensure the lowest positional number of any substituents. There are two substituents; the methoxy (-OMe) and aminomethyl (NH_2CH_2-) groups are at carbons-2 and -4, respectively.



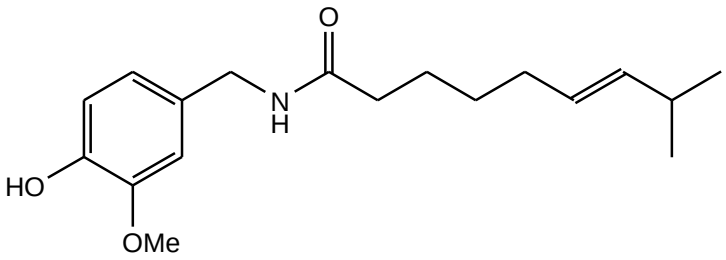
4-(aminomethyl)-2-methoxyphenol

3. This molecule is 4-(aminomethyl)-2-methoxyphenol. [Remember **a**minomethyl comes before **m**ethoxy as **a** comes before **m** in the alphabet.]

Answer

4-(aminomethyl)-2-methoxyphenol

(f) Name all of the functional groups in capsaicin.

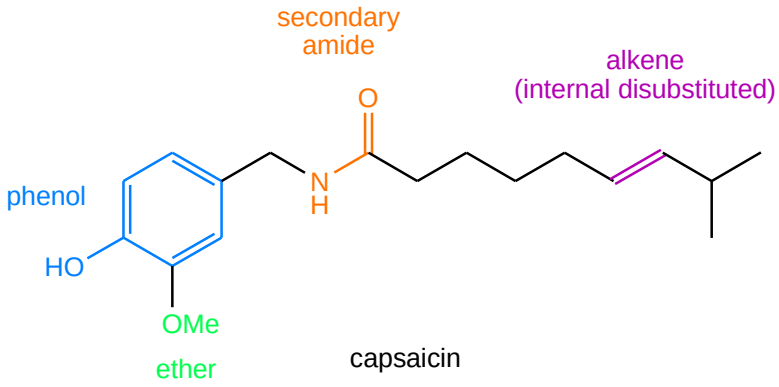


capsaicin

Strategy

This molecule contains four functional groups. There are three obvious functional groups, the ether group (ArOMe), the secondary amide (RCO_2NHR) and the substituted phenol (ArOH). The remaining functional group is an alkene.

Solution



capsaicin

Answer

Capsaicin contains FOUR functional groups; phenol, ether, secondary amide and alkene.

Solutions provided by J. Eames (j.eames@hull.ac.uk)