IUPAC Nomenclature

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IUPAC Nomenclature

The name of every organic molecule has 3 parts:

1. **The parent name indicates the number of carbons in the longest continuous chain.**
2. **The suffix indicates what functional group is present.**
3. **The prefix tells us the identity, location, and number of substituents attached to the carbon chain.**

Parent – Longest straight carbon chain

TABLE 4.1 Summary: Straight-Chain Alkanes

Number of C atoms	Molecular formula	Name (*n*-alkane)	Number of constitutional isomers
1	CH_4	methane	—
2	C_2H_6	ethane	—
3	C_3H_8	propane	—
4	C_4H_{10}	butane	2
5	C_5H_{12}	pentane	3
6	C_6H_{14}	hexane	5
7	C_7H_{16}	heptane	9
8	C_8H_{18}	octane	18
9	C_9H_{20}	nonane	35
10	$C_{10}H_{22}$	decane	75
20	$C_{20}H_{42}$	eicosane	366,319

Suffix – Our first functional group is alkane, so the suffix is –ane
For later functional groups we will drop the –ane root suffix for others

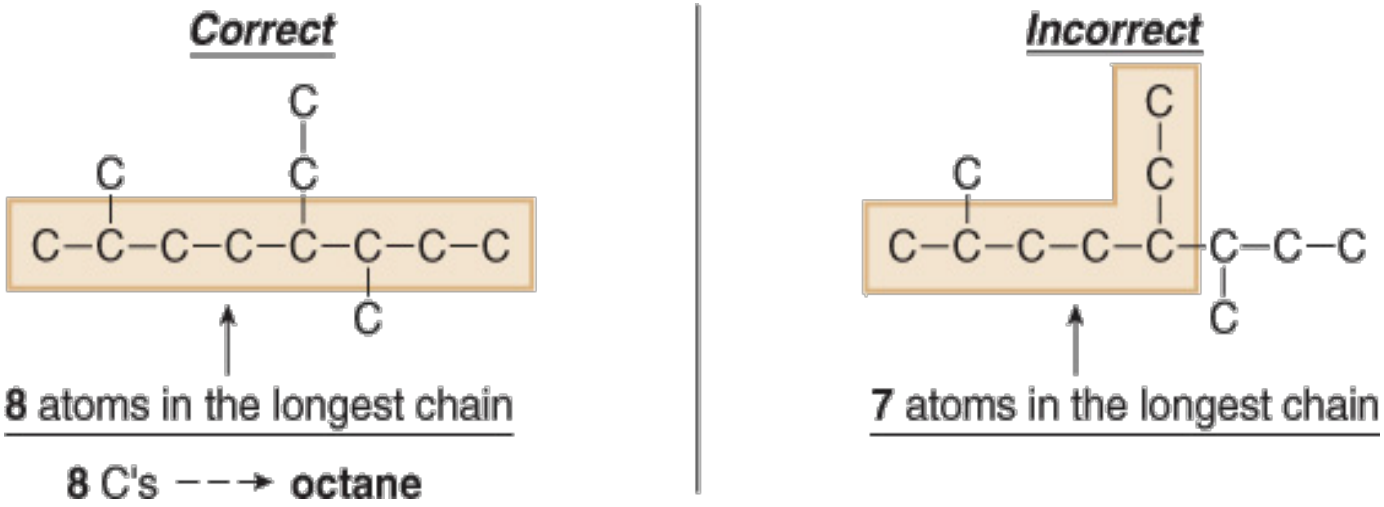
Alkane chain	# Carbons	Name
CH_4	1	methane
CH_3CH_3	2	ethane
$CH_3CH_2CH_3$	3	propane
$CH_3CH_2CH_2CH_3$	4	butane
$CH_3CH_2CH_2CH_2CH_3$	5	pentane
$CH_3CH_2CH_2CH_2CH_2CH_3$	6	hexane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	7	heptane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	8	octane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	9	nonane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	10	decane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	11	undecane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	12	dodecane

- **Prefix – Our substituents will be branches in the alkane structure**
  - **A branch is another alkane minus one hydrogen – an alkyl group**
  - **Example – if CH_3- is a branch on a longer chain:**
  - **CH_3- is CH_4 minus 1 hydrogen**
    - **Since it is a side chain it will replace the –ane suffix with –yl**
    - **CH_3- is a methyl group**
    - **We can also abbreviate this group as Me-**

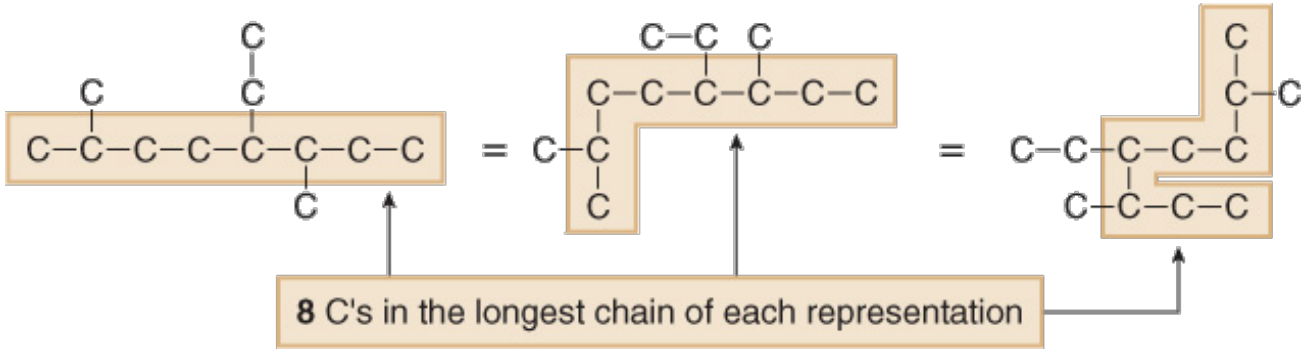
Prefixes -

Alkyl group	Structure	IUPAC name	Abbreviation
CH_3-	CH_3-	methyl	Me-
CH_3CH_2-		ethyl	Et-
$CH_3CH_2CH_2$-		*n*-propyl	*n*-Pr
CH_3CHCH_3		isopropyl or *i*-propyl	*i*-Pr
$CH_3CH_2CH_2CH_2$-		*n*-butyl	*n*-Bu
$CH_3CH_2CHCH_3$		*sec*-butyl	*s*-Bu
$(CH_3)_2CHCH_2$-		isobutyl or *i*-butyl	*i*-Bu
$(CH_3)_3C$-		*tert*-butyl or *t*-butyl	*t*-Bu
C_6H_5-		phenyl	Ph

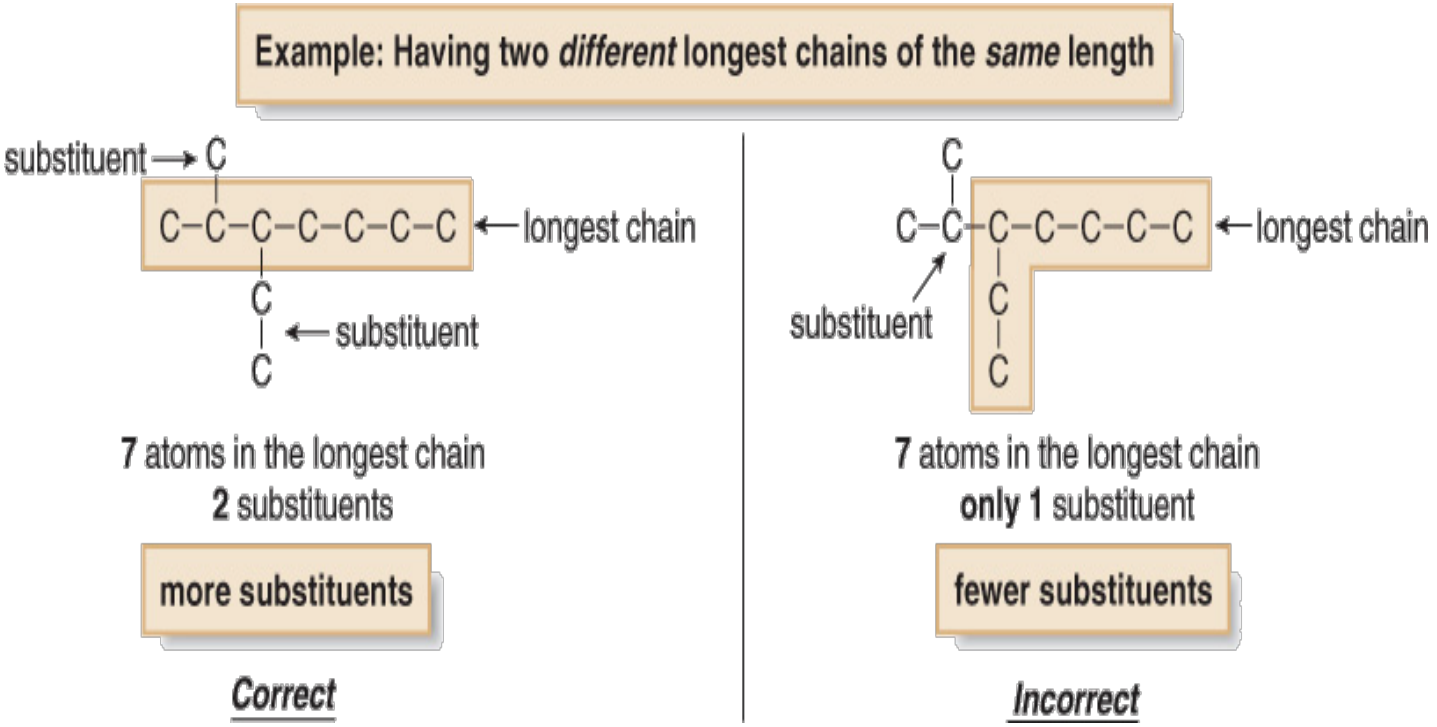
Find the parent carbon chain and add the suffix.



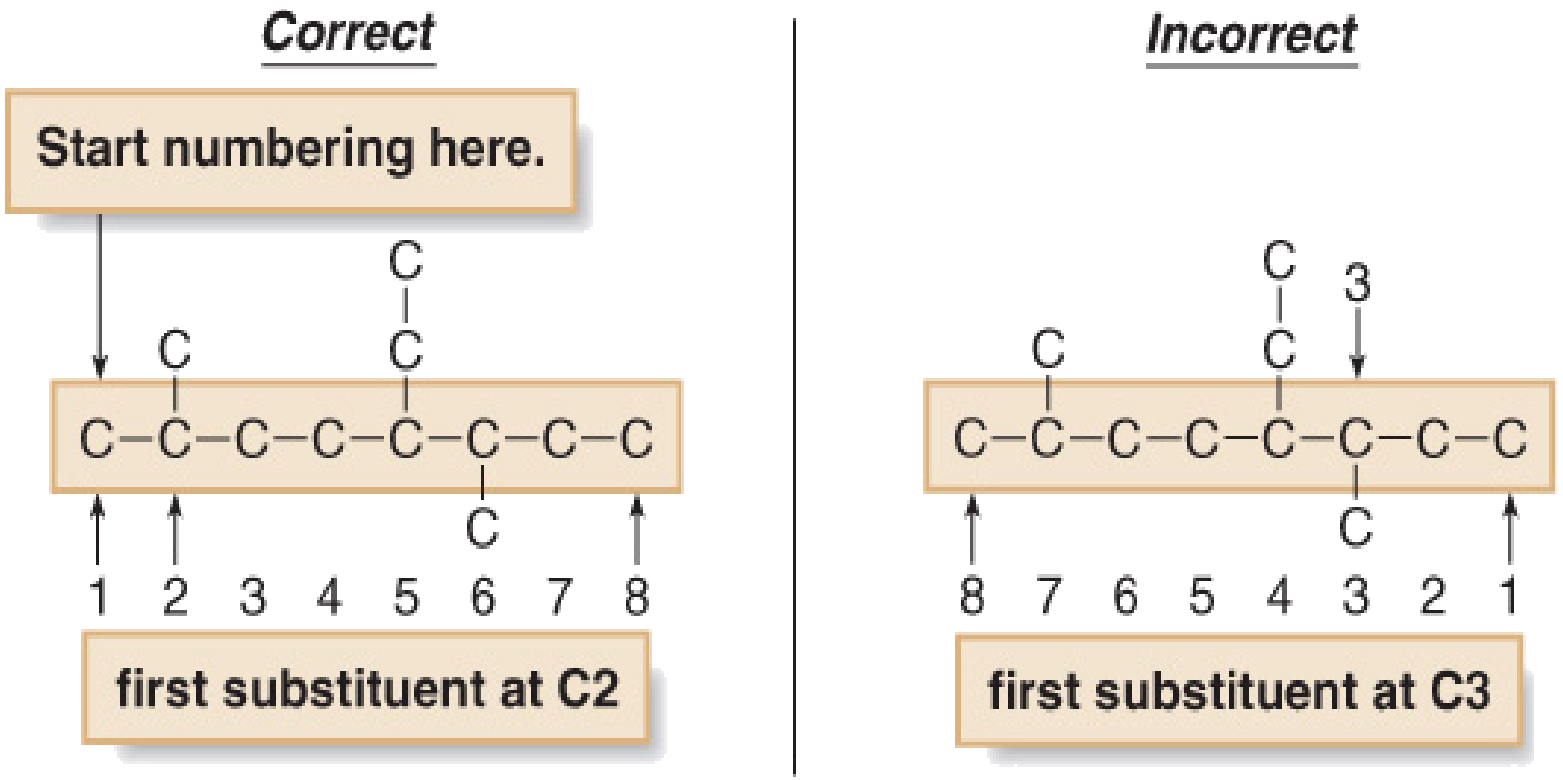
Note that it does not matter if the chain is straight or it bends.



Also note that if there are two chains of equal length, pick the chain with more substituents. In the following example, two different chains in the same alkane have seven C atoms. We circle the longest continuous chain as shown in the diagram on the left, since this results in the greater number of substituents.



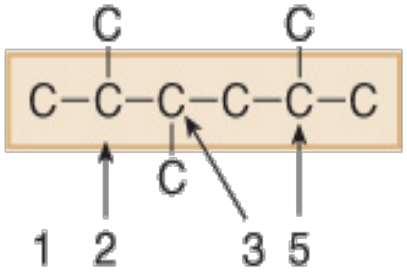
Number the atoms in the carbon chain to give the first substituent the lowest number.



If the first substituent is the same distance from both ends, number the chain to give the second substituent the lower number.

Example: Giving a lower number to the *second* substituent

Numbering from *left* to right

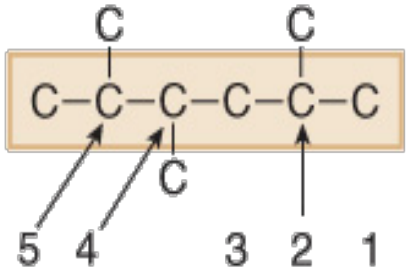


CH_3 groups at C2, **C3,** and C5.

The second substituent has a lower number.

Correct

Numbering from *right* to left

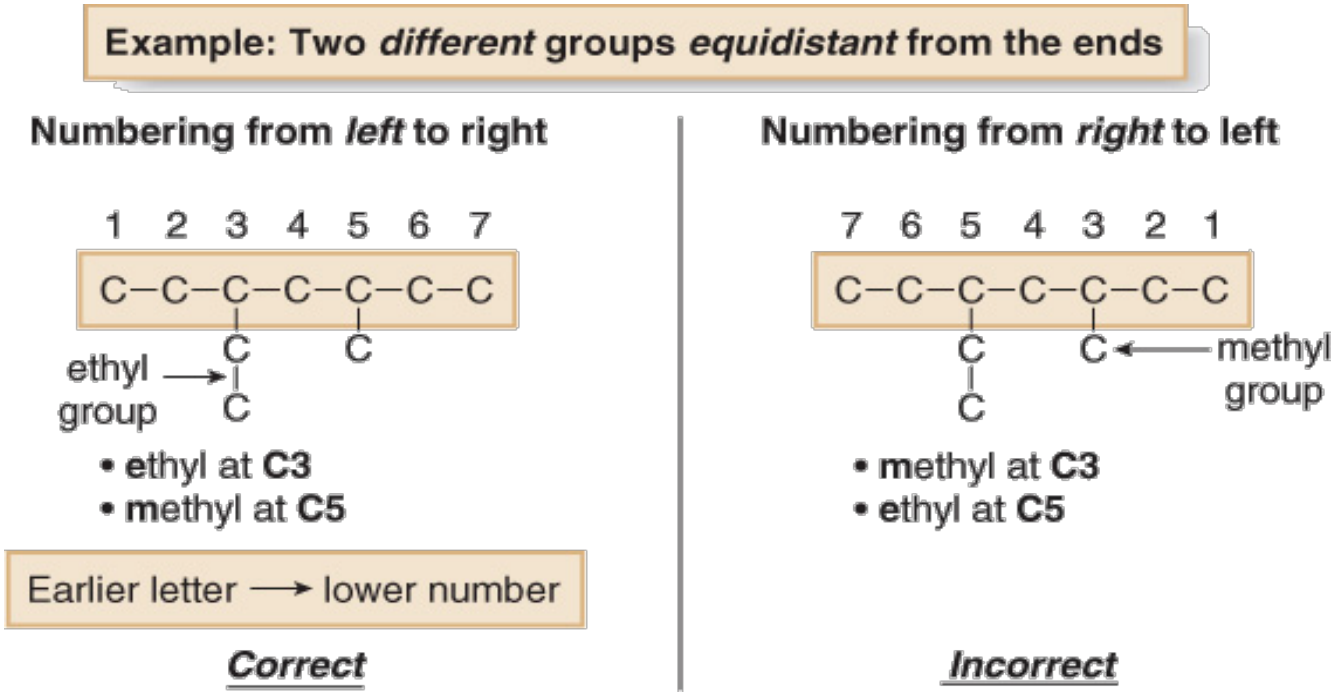


CH_3 groups at C2, **C4,** and C5.

higher number

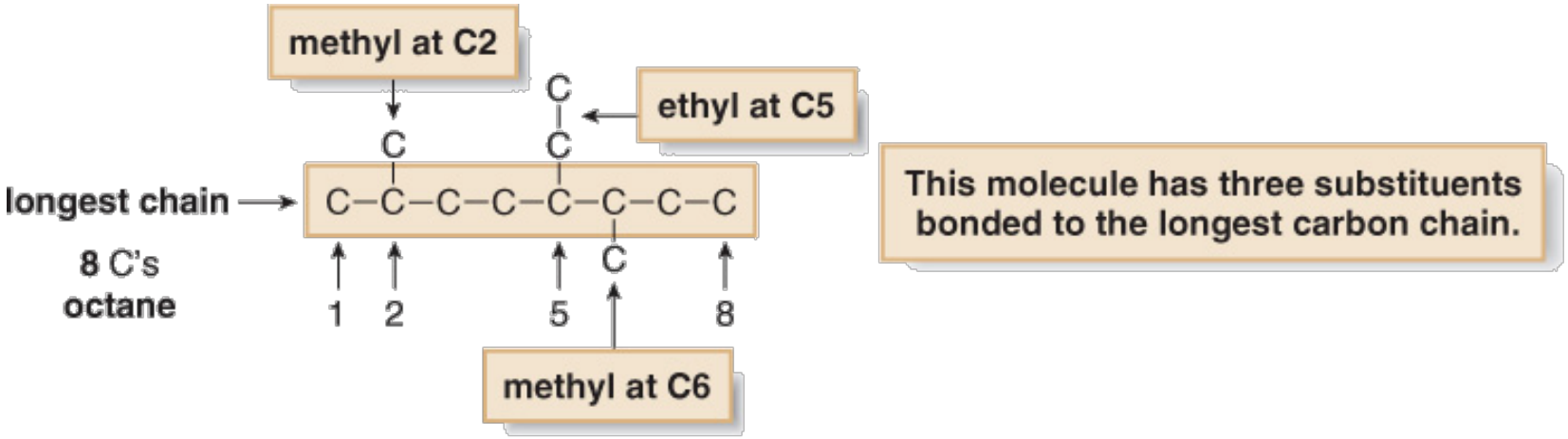
Incorrect

When numbering a carbon chain results in the same numbers from either end of the chain, assign the lower number alphabetically to the first substituent.



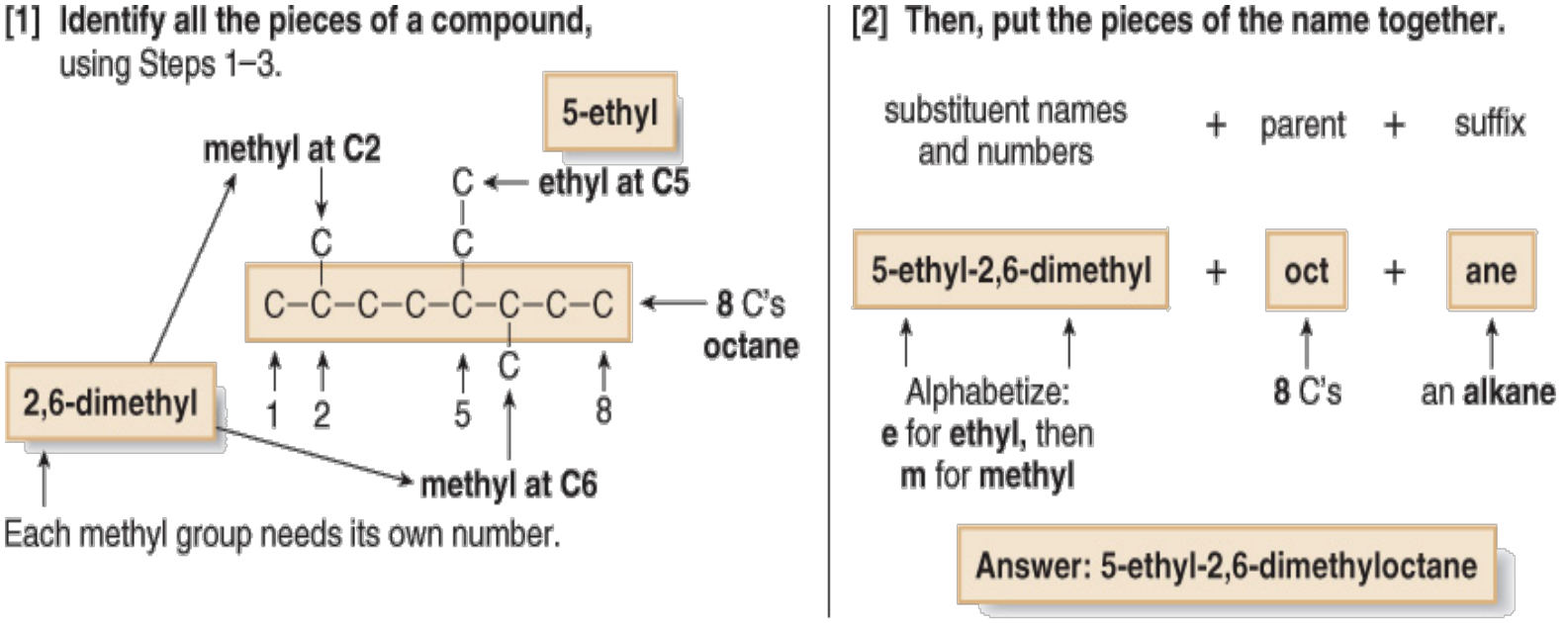
Name and number the substituents.

- Name the substituents as alkyl groups.
- Every carbon belongs to either the longest chain or a substituent, not both.
- Each substituent needs its own number
- If two or more identical substituents are bonded to the longest chain, use prefixes to indicate how many: di- for two groups, tri- for three groups, tetra- for four groups, and so forth.



Combine substituent names and numbers + parent and suffix.

- Precede the name of the parent by the names of the substituents.
- Alphabetize the names of the substituents, ignoring all prefixes except iso, as in isopropyl and isobutyl.
- Precede the name of each substituent by the number that indicates its location.
- Separate numbers by commas and separate numbers from letters by hyphens. The name of an alkane is a single word, with no spaces after hyphens and commas.



Thank You