

IUPAC Nomenclature: Machines Do It Better

Historically, the systematic naming of a compound was important in order to uniquely identify it and record relevant information about that compound. Today, computers are able to read and interpret graphical drawings of chemical structures; thus, the skill to name a compound no longer carries the importance that it once did. In the MarvinSketch example below, the program is being used to find the formal name of a tetrapropylene alkylbenzene sulfonate, a compound that once was used in laundry detergent. The IUPAC name is circled in the purple oval. **Today, it is far more important that you have the ability to use these tools and interpret their results rather than be an aficionado of IUPAC nomenclature.**

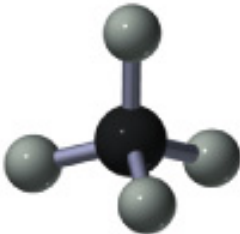
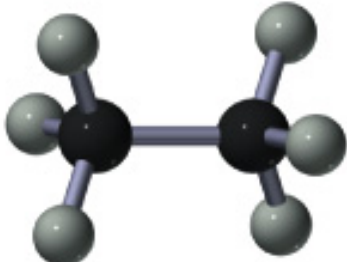
The image shows a screenshot of the MarvinSketch software interface. On the left, a chemical structure of a tetrapropylene alkylbenzene sulfonate is displayed. A dialog box titled "IUPAC Name Options" is open, showing the "Preferred IUPAC Name" option selected. On the right, a separate window titled "IUPAC Name" displays the preferred IUPAC name: **4-(2,4,6,7-tetramethyloctan-3-yl)benzenesulfonic acid**, which is circled in a purple oval. Below the name is a skeletal structure of the compound with methyl groups labeled as CH₃. A QR code is located in the bottom right corner, and a URL is provided at the bottom: http://www.chemaxon.com/anim/marvin/sketch_graphics/iupac.html

The Language of Chemistry

Hydrocarbons are compounds composed of only carbon and hydrogen

Alkanes are hydrocarbons containing only **single** bonds

The straight-chain n-alkanes: homologs of the series $\text{H}-(\text{CH}_2)_n-\text{H}$ whose molecular formula is represented by $\text{C}_n\text{H}_{2n+2}$.

| carbon number | name | Kekulé structure | condensed structure | ball-and-stick model |
|---------------|---------|--|--------------------------|---|
| C_1 | methane | $\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$ | CH_4 |  |
| C_2 | ethane | $\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$ | CH_3CH_3 |  |

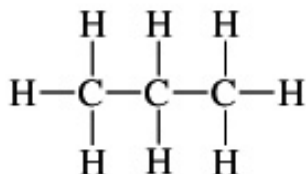
The Normal Alkanes

C₃ and C₄

carbon
number

C₃

propane

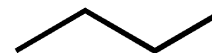
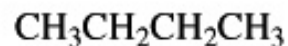
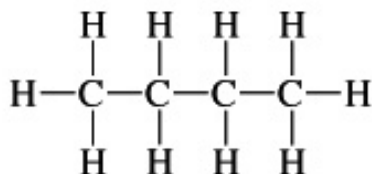


skeletal structure



C₄

butane



The skeletal structure shows the carbon-carbon bonds as lines and does not show the carbon-hydrogen bonds

The Normal Alkanes

$C_5 - C_{12}$

