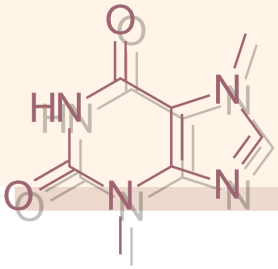
Theobromine

$C_7H_8N_4O_2$ Structure

Bond Angles
- Trigonal Planar | ~120°
- Tetrahedral | ~109°
- Trigonal Pyramidal | ~109°

Hybridization
- Trigonal Planar | sp^2
- Tetrahedral | sp^3
- Trigonal Pyramidal | sp^3



Molecular Formula
- $C_7H_8N_4O_2$

Sigma/Pi Bonding
- Total: 18 single, 4 double bonds
- 22 sigma bonds
- 4 pi bonds

Functional Groups
- 2 amine groups
- 2 amide groups
- 2 methyl groups
- 1 alkene group
- 1 imine group

Nomenclature

Common Name: theobromine

IUPAC: 3,7-dimethylxanthine-2,6-dione

Did You Know?

In a group of women that weigh 60kg, about half would die of theobromine poisoning after eating 19 pounds of chocolate in which 30g of theobromine can be found, or 7,084 Hershey's Kisses.

Sources and Uses

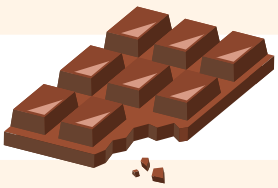
Sources

Theobromine is the primary purine alkaloid found in the cacao bean and (in trace amounts) in other plants including the yerba mate, kola nut, and guarana. However, the most common source of theobromine would be from the seeds of the theobroma cacao tree; it is extracted from the hulls of cacao beans. These beans contain approximately 1% theobromine.

Uses

The xanthine alkaloid and its salts/derivatives were can be used as bronchodilators and vasodilators, as well as a diuretic, myocardial stimulant, and smooth muscle relaxant.

Nowadays, small amounts of theobromine are often used in cooking and foods. It can be found in baked goods (avg. 345 ppm), frosting (avg. 1145 ppm), gelatins and puddings (avg. 300 ppm), milk products (avg. 480 ppm), and soft candy (avg. 1410 ppm).



General Information

Theobromine is the main purine alkaloid in theobroma cacao (the cacao bean) but can also be found, in trace amounts, in plants such as the guarana and yerba mate. Its stimulant effect is about 10x weaker than that of caffeine's, a molecule very similar in structure to theobromine. The bitterness of theobromine is what gives dark chocolate its taste.

State of Matter
As a solid:
- White, crystalline powder
- Bitter taste

Molar Mass
- 180.167 g/mol

Acidity
- Weakly acidic
- Combines with bases to form salts

Solubility
- Insoluble in water but soluble in organic solvents like ethanol

Reactivity/Fire Hazard
- Probably combustible (no data)
- May be sensitive to long exposure in light

Theobromine Poisoning

- CNS excitation
- Vomiting
- Nausea
- Tachycardia (condition that speeds up heart rate)
- Thirst
- Diarrhea
- Headache (in humans)

Consumption of theobromine does not affect humans to a great extent but small doses can be lethal for most animals.

LD_{50}
Humans, Rats, Mice:
- 1000mg/kg

Dogs:
- 300mg/kg

Cats:
- 200mg/kg

Health Hazards
In Humans & Animals

For humans, consuming large amounts of theobromine leads to vomiting and loss of appetite, as well as CNS and gastrointestinal upset.

Animals who consume theobromine may experience theobromine poisoning because their system does not metabolize theobromine as fast. However, significant poisoning rarely develops in humans.