CAFFEINE (ANHYDROUS)
Product Number C0750
Storage Temperature RT

CAS #: 58-08-2
Synonyms: 1,3,7-trimethylxanthine;
Methyltheobromine; 3,7-dihydro-1,3,7-trimethyl-1H-
purine-2,6-dione

![Chemical Structure of Caffeine]

Product Description
Appearance: white powder
Molecular Formula: C$_8$H$_{10}$N$_4$O$_2$
Molecular Weight: 194.2
Melting point: 238°C
Sublimes above 178°C at atmospheric pressure, but will sublimate at 160-165°C at 1 mm Hg
Extensive analytical data have been published. It's molecular weight is 194.2, its melting point is 238°C, and it sublimes above 178°C at atmospheric pressure, but will sublimate at 160-165°C at 1 mm Hg.

The product is synthetic, prepared according to the Taub synthesis method.

A popular central nervous system (CNS) stimulant. Caffeine is a well-known drug commonly used as a mild stimulant, found in dietary sources such as coffee, tea, and cocoa. It is believed to act through adenosine receptors and monoamine neurotransmitters. It is an adenosine receptor antagonist and adenosine 3',5'-cyclic monophosphate (cAMP) phosphodiesterase inhibitor. Thus, levels of cAMP increase in cells following treatment with caffeine. It has been reported to affect cellular calcium levels, releasing calcium from intracellular stores. It overrides the cell cycle effects of various chemicals such as protease inhibitors, thereby preventing apoptosis, and it has been shown to inhibit cellular DNA repair mechanisms.

Precautions and Disclaimer
Keep tightly sealed.

Preparation Instructions
The solubility in ethanol is 1 g in 66 ml (approx. 15 mg/ml). Caffeine is also soluble in water (approx. 16 mg/ml at room temperature, 200 mg/ml at 80°C, or 666 mg/ml in boiling water. Solubility in water is increased by adding dilute acid (e.g. HCl or citric acid). Caffeine is decomposed by strong bases.

Storage/Stability
Stored at room temperature this product has a shelf-life of 4 years. Solutions in organic solvents (e.g. methanol or ethanol) are stable at 2-8°C for several years.

References
5. Sigma quality control data.
6. Supplier information.

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