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ProductInformation

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

Product Description

Appearance: white powder Molecular Formula: C₈H₁₀N₄O₂ Molecular Weight: 194.2 Melting point: 238°C¹

Sublimes above 178°C at atmospheric pressure, but

will sublime at 160-165°C at 1 mm Hg Extensive analytical data have been published.²⁻⁴

 $pK_{a} = 14.0 \text{ at } 25^{\circ}C^{4}$

 $E^{mM}(272 \text{ nm}) = 9.3-9.4 (0.1 \text{ M HCl})^5$

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 12-14; 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. ⁵

References

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