

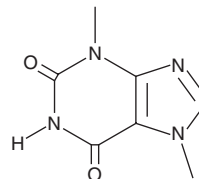
PRODUCT INFORMATION



Theobromine

Item No. 21745

CAS Registry No.: 83-67-0
Formal Name: 3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione
Synonyms: Diurobromine, NSC 5039, SC-15090
MF: C₇H₈N₄O₂
FW: 180.2
Purity: ≥98%
UV/Vis.: λ_{max}: 273 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Theobromine is supplied as a crystalline solid. A stock solution may be made by dissolving the theobromine in the solvent of choice, which should be purged with an inert gas. Theobromine is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of theobromine in these solvents is approximately 0.5, 30, and 20 mg/ml, respectively.

Theobromine is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, theobromine should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Theobromine has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Theobromine is a methylxanthine alkaloid and derivative of caffeine (Item No. 14118) that has been found in cocoa beans and has diverse biological activities.¹⁻³ It is an adenosine A₁ receptor antagonist (IC₅₀s = 200-280 μM in radioligand binding assays using rat brain membranes).² Theobromine (150 μg/ml) increases AMPK phosphorylation and inhibits adipocyte differentiation, ERK and JNK phosphorylation, and IL-6 and TNF-α production in 3T3-L1 preadipocytes cultured in differentiation medium.¹ It inhibits decreases in renal cortex SIRT1 activity and increases in NADPH oxidase-dependent reactive oxygen species (ROS) production, as well as reduces kidney hypertrophy and albuminuria in a spontaneously hypertensive rat model of streptozotocin-induced diabetes when administered at a dose of 5 mg/kg per day.³ Theobromine is toxic to dogs with an LD₅₀ value of 250 to 500 mg/kg.⁴

References

1. Jang, Y.J., Koo, H.J., Sohn, E.-H., *et al.* Theobromine inhibits differentiation of 3T3-L1 cells during the early stage of adipogenesis via AMPK and MAPK signaling pathways. *Food Funct.* **6**(7), 2365-2374 (2015).
2. Daly, J.W., Butts-Lamb, P., and Padgett, W. Subclasses of adenosine receptors in the central nervous system: Interaction with caffeine and related methylxanthines. *Cell. Mol. Neurobiol.* **3**(1), 69-80 (1983).
3. Papadimitriou, A., Silva, K.C., Peixoto, E.B.M.I., *et al.* Theobromine increases NAD⁺/Sirt-1 activity and protects the kidney under diabetic conditions. *Am. J. Physiol. Renal Physiol.* **308**(3), F209-F225 (2015).
4. Lawrence, L.P. Chocolate toxicosis. *The 5-minute veterinary consult: Canine and feline.* Smith, F.W.K. Jr., editor, 3rd ed., Lippincott Williams & Wilkins (2004).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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