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Product Information

Cat. No. B4147
BENZOYLECGONINE HYDRATE--DEA SCHEDULE II

Cocaine metabolite.

Mol. Formula: C₁₆H₁₉NO₄

Mol. Wt.: 289.33 (anhyd.)

m.p.: 198-200°C

CAS Registry No.: 519-09-5

Chemical Name: 3β-Hydroxy-1αH,5αH-tropane-2β-carboxylic acid benzoate

Physical Properties: White solid. $[\alpha]_D^{22} = -48.66^\circ$ (c = 1.2, H₂O).

Caution: The pharmacology of this compound is incompletely characterized and due care should be exercised in its use. Avoid skin contact, ingestion or inhalation.

Storage: Store tightly sealed at -20°C.

Solubility: Soluble in ethanol or 1M NaHCO₃ (>26.4 mg/ml); insoluble in water.

Disposal: Dissolve or mix the compound with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. This product is controlled by the Drug Enforcement Administration. Appropriate security must be maintained until the substance is destroyed. Records must be kept which detail the ultimate disposition of the material.

References:

1. *Merck Index 11th Ed.*, No. 1125.
2. Barbieri, E.J., Ferko, A.P., DiGregorio, G.J., Ruch, E.K. "The presence of cocaine and benzoylecgonine in rat cerebrospinal fluid after the intravenous administration of cocaine." *Life Sci.* **51**, 1739-1746 (1992).
3. Ambre, J., Ruo, T.I., Nelson, J., Belknap, S. "Urinary excretion of cocaine, benzoylecgonine, and ecgonine methyl ester in humans." *J. Anal. Toxicol.* **12**, 301-306 (1988).
4. Lau, C.E., Ma, F., Falk, J.L. "Simultaneous determination of cocaine and its metabolites with caffeine in rat serum microsomes by high-performance liquid chromatography." *J. Chromatogr.* **532**, 95-103 (1990).

CONTROLLED SUBSTANCE - DEA LICENSE REQUIRED (II)

Rev. 1/96

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