



Product Information

Cat. No. C0932
COCAETHYLENE--DEA SCHEDULE II
ETHYLBENZOYLECGONINE HYDROCHLORIDE;
COCAINE ETHYL ESTER HYDROCHLORIDE

>99% purity

Analog of cocaine which has been detected in the urine of simultaneous cocaine and ethanol abusers.

Mol. Formula: C₁₈H₂₃NO₄·HCl

Mol. Wt.: 353.85 (anhyd.)

m.p.: 105-145°C (for mixed hydrate)

CAS Registry No.: 529-38-4

Chemical Name: (-)-2β-Carboethoxy-3β-benzoyloxytropane hydrochloride

Physical Properties: White hygroscopic solid; $[\alpha]_D^{25} = -56.2^\circ$ (c = 1.55, 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. RTECS No. CL5602980.

Storage: Store desiccated at room temperature.

Solubility: Soluble 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. Rafla, F.K., Epstein, R.L. "Identification of cocaine and its metabolites in human urine in the presence of ethyl alcohol." *J. Anal. Toxicol.* **3**, 59-63 (1979).
2. Lukaszewski, T., Jeffery, W.K. "Impurities and artifacts of illicit cocaine." *J. Forensic. Sci.* **25**, 499-507 (1980).
3. Smith, R.M. "Ethyl esters of arylhydroxy- and arylhydroxymethoxycocaines in the urines of simultaneous cocaine and ethanol users." *J. Anal. Toxicol.* **8**, 38-42 (1984).

Sigma-RBI brand products are sold through Sigma-Aldrich, Inc.

Sigma-Aldrich, Inc. warrants that its products conform to the information contained in this and other Sigma-Aldrich publications.

Purchaser must determine the suitability of the product(s) for their particular use. Additional terms and conditions may apply.

Please see reverse side of the invoice or packing slip.

4. Hearn, W.L., Flynn, D.D., Hime, G.W., Rose, S., Cofino, J.C., Mantero-Atienza, E., Wetli, C.V., Mash, D.C. "Cocaethylene: A unique cocaine metabolite displays high affinity for the dopamine transporter." *J. Neurochem.* **56**, 698-701 (1991).
5. Jatlow, P., Elsworth, J.D., Bradberry, C.W., Winger, G., Taylor, J.R., Russell, R., Roth, R.H. "Cocaethylene: A neuropharmacologically active metabolite associated with concurrent cocaine-ethanol ingestion." *Life Sci.* **48**, 1787-1794 (1991).
6. Lau, C.E. "Determination of cocaethylene, cocaine and their metabolites in rat serum microsamples by high-performance liquid chromatography, and its application to pharmacokinetic studies in rodents." *J. Chromatogr.* **582**, 167-172 (1992).

CONTROLLED SUBSTANCE - DEA LICENSE REQUIRED (II)

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