Safety Data Sheet

SAFETY DATA SHEET - LC LABORATORIES REVISION DATE: JULY 1, 2019

SECTION 1. IDENTIFICATION:

Trade name: CI-994, Free Base

Product Number: C-2606 Manufacturer/Supplier:

LC Laboratories

165 New Boston Street Woburn, MA 01801 USA

1-781-937-0777 Fax: 1-781-938-5420

SECTION 2. HAZARD(S) IDENTIFICATION:

Hazard Description: Harmful

Substance Class Identifier: Drug; Human Data

Ingestion may cause adverse gastrointestinal, blood, and reproductive effects including suppression of bone marrow function, changes in thymus function, thrombocytopenia (low platelet count), leukopenia (low white blood cell count), anemia, diarrhea, dehydration, loss of appetite, degeneration of the testes, and possible risk of impaired fertility

Has been shown to cause chromosomal damage in certain mammalian cells Exposure causes eye irritation; exposure may cause irritation of the skin, mucous membranes, and upper respiratory tract

Signal Word: Harmful

GHS Hazard Statements:

H302+312+332 - Harmful if swallowed, in contact with skin or if inhaled

GHS Precautionary Statements:

P2562 - Do not get in eyes, on skin or on clothing WARNING: For Laboratory Research Use Only

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS:

Chemical Name: 4-(Acetylamino)-N-(2-aminophenyl)benzamide

Synonyms: Acetyldinaline, Goe 5549, Gö 5549, PD 123654, Tacedinaline

Hazardous Ingredient: CI-994, Free Base

CAS Registry Number: 112522-64-2

Molecular Weight: 269.30

Molecular Formula: $C_{15}H_{15}N_3O_2$

SECTION 4. FIRST-AID MEASURES:

After Inhalation: If inhaled, remove to fresh air; if breathing is difficult, give oxygen; if breathing stops, give artificial respiration

After skin contact: flush with copious amounts of water; remove contaminated clothing and shoes; call a physician

After eye contact: check for and remove contact lenses; flush with copious amounts of water; assure adequate flushing by separating the eyelids with fingers; call a physician

After swallowing: if swallowed, wash out mouth with copious amounts of water; call a physician

SECTION 5. FIRE-FIGHTING MEASURES:

Suitable extinguishing agents: water spray, carbon dioxide, dry chemical powder or foam

Protective equipment: wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes

Unusual fire hazard: may emit toxic fumes under fire conditions such as carbon monoxide, etc.

SECTION 6. ACCIDENTAL RELEASE MEASURES:

Person-related safety precautions: cordon off area of spill; wear self-contained breathing apparatus, protective clothing and heavy rubber gloves Measures for cleaning/collecting: absorb solutions with finely- powdered liquid-binding material (diatomite, universal binders); decontaminate surfaces and equipment by scrubbing with alcohol; dispose of contaminated material according to Section 13

SECTION 7. HANDLING AND STORAGE:

Information for safe handling: avoid contact with skin, eyes and clothing; material may be an irritant

Storage: store solid and solutions at -20 °C

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION:

Personal protective equipment as follows:

Breathing equipment: NIOSH/MSHA-approved respirator

Protection of hands: handle with Nitrile rubber gloves with minimum thickness of 0.11 mm (4.3 mil). This recommendation should not be interpreted as offering an approval for any specific use conditions. Please review this recommendation with a safety officer to evaluate if it is appropriate for the anticipated use.

Eye protection: chemical safety goggles

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES:

Page 3 of 4

Form: crystalline solid; granular or powder

Color: white to off-white

Odor: none

Melting point/Melting range: 233-243 °C

Danger of explosion: none

Solubility in / Miscibility with water: very poorly soluble in water; maximum solubility in plain water is estimated to be about 25-100 μ M; buffers, serum, or

other additives may increase or decrease the aqueous solubility

Solvent content:

Organic solvents: soluble in DMSO at 66 mg/mL; very poorly soluble in ethanol

SECTION 10. STABILITY AND REACTIVITY:

Stability: avoid acids and bases

Thermal decomposition / conditions to be avoided: protect from light and heat Dangerous products of decomposition: thermal decomposition may produce toxic gases such as carbon monoxide and carbon dioxide, and nitrogen oxides

SECTION 11. TOXICOLOGICAL INFORMATION:

RTECS #: CU8702023

Acute toxicity: oral toxicity (TDLo): 70-700 mg/kg (mouse), 14 mg/kg (dog);

intravenous toxicity (LD50): 0.7 mg/kg (human)

Primary irritant effect: not known

On the skin: may be an irritant; may be harmful if absorbed through the skin

On the eye: causes eye irritation

Inhalation: may be harmful if inhaled; may cause respiratory tract irritation

Ingestion: harmful if swallowed

SECTION 12. ECOLOGICAL INFORMATION:

General notes: no data available

Treat as potentially toxic if released into the environment

SECTION 13. DISPOSAL CONSIDERATIONS:

Dispose of in accordance with prevailing country, federal, state and local regulations

SECTION 14. TRANSPORT INFORMATION:

UN number: 2811

DOT: Toxic solid, organic, n.o.s. (4-(Acetylamino)-*N*-(2-aminophenyl)benzamide), Class: 6.1, Packing group: III IMDG: Toxic solid, organic, n.o.s. (4-(Acetylamino)-*N*-(2-aminophenyl)benzamide), Class: 6.1, Packing group: III IATA: Toxic solid, organic, n.o.s. (4-(Acetylamino)-*N*-(2-aminophenyl)benzamide), Class: 6.1, Packing group: III

SECTION 15. REGULATORY INFORMATION:

Code letter and hazard designation of product:

Xn: Harmful

EU Risk And Safety phrases: S22: Do not breathe dust

S36/37: Wear suitable protective clothing and gloves

S45: In case of accident or if you feel unwell, seek medical advice immediately (show label where possible)

S53: Avoid exposure-obtain special instructions before use

R22: Harmful if swallowed

R48/22: Harmful: danger of serious damage to health by prolonged exposure if

swallowed

R62: Possible risk of impaired fertility

SECTION 16. OTHER INFORMATION:

The above information is believed to be correct based on our present knowledge but does not purport to be complete. For research use only by trained personnel. The burden of safe use of this material rests entirely with the user. LC Laboratories disclaims all liability

Reviewed: July 1, 2019