

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 1272/2008

Section 1. Identification of the Substance/Mixture and of the Company/Undertaking

- 1.1 Product Code:** 14153
Product Name: Entacapone
Synonyms: 2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethyl-2E-propenamide; Comtan; OR 611;
- 1.2 Relevant identified uses of the substance or mixture and uses advised against:**
Relevant identified uses: For research use only, not for human or veterinary use.
- 1.3 Details of the Supplier of the Safety Data Sheet:**
Company Name: Cayman Chemical Company
 1180 E. Ellsworth Rd.
 Ann Arbor, MI 48108
Web site address: www.caymanchem.com
Information: Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**
Emergency Contact: CHEMTREC Within USA and Canada: +1 (800)424-9300
 CHEMTREC Outside USA and Canada: +1 (703)527-3887

Section 2. Hazards Identification

- 2.1 Classification of the Substance or Mixture:**
2.1.1 Classification according to Regulation (EC) No 1272/2008 [CLP]:
 Skin Corrosion/Irritation, Category 2
 Serious Eye Damage/Eye Irritation, Category 2A
 Target Organ Systemic Toxicity (single exposure), Category 3
2.1.2 Classification according to Directive 1999/45/EC:
 Xi: Irritant
 Risk Phrases: R36/37/38
 For full text of R- phrases: see SECTION 15.
- 2.2 Label Elements:**
2.2.1 Labeling according to Regulation (EC) No 1272/2008 [CLP]:



GHS Signal Word: Warning

GHS Hazard Phrases:

H315: Causes skin irritation.
 H319: Causes serious eye irritation.
 H335: May cause respiratory irritation.

GHS Precaution Phrases:

P264: Wash {hands} thoroughly after handling.
 P280: Wear {protective gloves/protective clothing/eye protection/face protection}.
 P362+364: Take off contaminated clothing and wash it before reuse.
 P261: Avoid breathing {dust/fume/gas/mist/vapours/spray}.

GHS Response Phrases:

P302+352: IF ON SKIN: Wash with plenty of soap and water.
 P332+313: If skin irritation occurs, get medical advice/attention.
 P305+351+338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P337+313: If eye irritation persists, get medical advice/attention.

P309+311: Call a POISON CENTER or doctor/physician if exposed or you feel unwell.

P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

GHS Storage and Disposal Phrases:

Please refer to Section 7 for Storage and Section 13 for Disposal information.

2.2.2 Labeling according to Directive 1999/45/EC:



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2.3 Adverse Human Health Causes skin irritation.

Effects and Symptoms: Causes serious eye irritation.

Material may be irritating to the mucous membranes and upper respiratory tract.

May be harmful by inhalation, ingestion, or skin absorption.

May cause respiratory irritation.

To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

Section 3. Composition/Information on Ingredients

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	Risk Phrases/ GHS Classification
130929-57-6 NA	Entacapone	100.0 %	603-449-6 NA	Xi; R36/37/38 Skin Corr. 2: H315 Eye Damage 2A: H319 TOST (SE) 3: H335 H336

Section 4. First Aid Measures

4.1 Description of First Aid Measures:

In Case of Inhalation: Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.

In Case of Skin Contact: Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

In Case of Eye Contact: Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined and tested by medical personnel.

In Case of Ingestion: Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.

Section 5. Fire Fighting Measures

5.1 Suitable Extinguishing Media: Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.

Media: Use water spray to cool fire-exposed containers.

Unsuitable Extinguishing Media: A solid water stream may be inefficient.

5.2 Flammable Properties and Hazards: No data available.

Flash Pt: No data.

Explosive Limits: LEL: No data. UEL: No data.

Autoignition Pt: No data.

5.3 Fire Fighting Instructions:	As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.
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Section 6. Accidental Release Measures

6.1 Protective Precautions, Protective Equipment and Emergency Procedures:	Avoid raising and breathing dust, and provide adequate ventilation. As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator, and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
6.2 Environmental Precautions:	Take steps to avoid release into the environment, if safe to do so.
6.3 Methods and Material For Containment and Cleaning Up:	Contain spill and collect, as appropriate. Transfer to a chemical waste container for disposal in accordance with local regulations.

Section 7. Handling and Storage

7.1 Precautions To Be Taken in Handling:	Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure.
7.2 Precautions To Be Taken in Storing:	Keep container tightly closed. Store in accordance with information listed on the product insert.

Section 8. Exposure Controls/Personal Protection

8.1 Exposure Parameters:

CAS #	Partial Chemical Name	Britain EH40	France VL	Europe
130929-57-6	Entacapone	No data.	No data.	No data.
CAS #	Partial Chemical Name	OSHA TWA	ACGIH TWA	Other Limits
130929-57-6	Entacapone	No data.	No data.	No data.

8.2 Exposure Controls:

8.2.1 Engineering Controls (Ventilation etc.):	Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.
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8.2.2 Personal protection equipment:

Eye Protection:	Safety glasses
Protective Gloves:	Compatible chemical-resistant gloves
Other Protective Clothing:	Lab coat
Respiratory Equipment (Specify Type):	NIOSH approved respirator, as conditions warrant.
Work/Hygienic/Maintenance Practices:	Do not take internally. Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower. Wash thoroughly after handling.

Section 9. Physical and Chemical Properties

9.1 Information on Basic Physical and Chemical Properties

Physical States: ☐ Gas ☐ Liquid ☒ Solid
Appearance and Odor: A crystalline solid
Melting Point: No data.
Boiling Point: No data.
Flash Pt: No data.
Evaporation Rate: No data.
Explosive Limits: LEL: No data. UEL: No data.
Vapor Pressure (vs. Air or mm Hg): No data.
Vapor Density (vs. Air = 1): No data.
Specific Gravity (Water = 1): No data.
Solubility in Water: No data.
Solubility Notes: ~0.5 mg/ml in 1:1 DMSO:PBS (pH 7.2); ~5 mg/ml in EtOH; ~30 mg/ml in DMSO & DMF;
Autoignition Pt: No data.

9.2 Other Information

Percent Volatile: No data.
Molecular Formula & Weight: C₁₄H₁₅N₃O₅ 305.3

Section 10. Stability and Reactivity

10.1 Reactivity: No data available.
10.2 Stability: Unstable ☐ Stable ☒
10.3 Stability Note(s): Stable if stored in accordance with information listed on the product insert.
Polymerization: Will occur ☐ Will not occur ☒
10.4 Conditions To Avoid: No data available.
10.5 Incompatibility - Materials To Avoid: No data available.
10.6 Hazardous Decomposition Or Byproducts: No data available.

Section 11. Toxicological Information

11.1 Information on Toxicological Effects: The toxicological effects of this product have not been thoroughly studied.
 Entacapone - Toxicity Data: Oral TDLO (rat): 10 mg/kg; Oral TDLO (rat): 140 mg/kg/7D (intermittent);
Chronic Toxicological Effects: Entacapone - Investigated as a mutagen, reproductive effector, and tumorigen. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information.
 Entacapone RTECS Number: UC6316195
Carcinogenicity: NTP? No IARC Monographs? No OSHA Regulated? No

Section 12. Ecological Information

12.1 Toxicity: Avoid release into the environment.
Runoff from fire control or dilution water may cause pollution.

Section 13. Disposal Considerations

13.1 Waste Disposal Method: Dispose in accordance with local, state, and federal regulations.

Section 14. Transport Information

14.1 LAND TRANSPORT (US DOT):

DOT Proper Shipping Name: Not dangerous goods.

DOT Hazard Class:

UN/NA Number:

14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name: Not dangerous goods.

UN Number:

Hazard Class:

14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Not dangerous goods.

Additional Transport Information: Transport in accordance with local, state, and federal regulations.

Section 15. Regulatory Information

EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
130929-57-6	Entacapone	No	No	No

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
130929-57-6	Entacapone	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No

European Community Hazard Symbol codes:



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European Community Risk and Safety Phrases:

R36/37/38 Irritating to eyes, respiratory system and skin.
S22 Do not breathe dust.
S24/25 Avoid contact with skin and eyes.
S36/37/39 Wear suitable protective clothing, gloves and eye/face protection.

Regulatory Information Statement: This SDS was prepared in accordance with Regulation (EC) No.1272/2008 and European Directive 67/548/EEC as amended.

Section 16. Other Information

Revision Date: 12/16/2013

Additional Information About No data available.

This Product:

Company Policy or

Disclaimer:

DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.

N.A.=Not available, N.P.=Not applicable, N.D.=Not determined, N.E.=Not established,
N.R.=Not required