SECTION 1. Identification

Product identifier

- Product number: 841629
- Product name: Phenylglyoxylic acid for synthesis

Relevant identified uses of the substance or mixture and uses advised against

- Identified uses: Chemical for synthesis
- Uses advised against:

Details of the supplier of the safety data sheet

- Company: EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | SDS Phone Support: +1-978-715-1335 | General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
- e-mail: mm_sds@merckgroup.com

Emergency telephone

- 613-996-6666 CANUTEC (Canada)
- +1-703-527-3887 CHEMTREC (International)
- 24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

- Skin irritation, Category 2, H315
- Eye irritation, Category 2, H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

GHS-Labeling

Hazard pictograms

- !

Signal Word

Warning

Hazard Statements

- H315 Causes skin irritation.
- H319 Causes serious eye irritation.
Precautionary Statements
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Other hazards
None known.

SECTION 3. Composition/information on ingredients

Formula: \((\text{C}_6\text{H}_5)\text{COCOOH}\)  \(\text{C}_8\text{H}_6\text{O}_3\) (Hill)
CAS-No.: 611-73-4
Molar mass: 150.13 g/mol

Hazardous ingredients

<table>
<thead>
<tr>
<th>Chemical Name (Concentration)</th>
<th>CAS-No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzoylformic acid (&gt;= 90 % - &lt;= 100 %)</td>
<td>611-73-4</td>
</tr>
</tbody>
</table>

SECTION 4. First aid measures

Description of first-aid measures

Inhalation
After inhalation: fresh air.

Skin contact
After skin contact: wash off with plenty of water. Remove contaminated clothing.

Eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist.

Ingestion
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed
irritant effects

Indication of any immediate medical attention and special treatment needed
No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media
Water, Carbon dioxide (CO2), Foam, Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.
Special hazards arising from the substance or mixture
   Combustible material, Development of hazardous combustion gases or vapors possible in the event of fire.

Advice for firefighters
   **Special protective equipment for fire-fighters**
   Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

   **Further information**
   Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

**Personal precautions, protective equipment and emergency procedures**
   Advice for non-emergency personnel: Avoid substance contact. Avoid generation of dusts; do not inhale dusts. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

   Advice for emergency responders: Protective equipment see section 8.

**Environmental precautions**
   Do not empty into drains.

**Methods and materials for containment and cleaning up**
   Cover drains. Collect, bind, and pump off spills.
   Observe possible material restrictions (see sections 7 and 10).
   Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. Handling and storage

**Precautions for safe handling**
   Observe label precautions.

**Conditions for safe storage, including any incompatibilities**
   Tightly closed. Dry.

   Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

**Exposure limit(s)**
   Contains no substances with occupational exposure limit values.

**Engineering measures**
   Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

**Individual protection measures**
   Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

**Hygiene measures**
   Immediately change contaminated clothing. Apply skin-protective barrier cream. Wash hands and face after working with substance.
Eye/face protection
Safety glasses

Hand protection
Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:
protective clothing

Respiratory protection
required when dusts are generated.
Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state</td>
<td>crystalline</td>
</tr>
<tr>
<td>Color</td>
<td>light cream</td>
</tr>
<tr>
<td>Odor</td>
<td>No strong odor known.</td>
</tr>
<tr>
<td>Odor Threshold</td>
<td>No information available.</td>
</tr>
<tr>
<td>pH</td>
<td>No information available.</td>
</tr>
<tr>
<td>Melting point</td>
<td>62 - 66 °C</td>
</tr>
<tr>
<td>Boiling point.boiling range</td>
<td>297 - 304 °F (147 - 151 °C) at 16 hPa</td>
</tr>
<tr>
<td>Flash point</td>
<td>No information available.</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No information available.</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No information available.</td>
</tr>
<tr>
<td>Lower explosion limit</td>
<td>No information available.</td>
</tr>
<tr>
<td>Upper explosion limit</td>
<td>No information available.</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>No information available.</td>
</tr>
<tr>
<td>Relative vapor density</td>
<td>No information available.</td>
</tr>
<tr>
<td>Relative density</td>
<td>1.38 g/cm³</td>
</tr>
<tr>
<td></td>
<td>at 68 °F (20 °C)</td>
</tr>
<tr>
<td>Water solubility</td>
<td>soluble</td>
</tr>
</tbody>
</table>
Partition coefficient: n-octanol/water
log Pow: 1.20 (calculated)
Bioaccumulation is not expected (log Pow <1). (Lit.)

Autoignition temperature
No information available.

Decomposition temperature
No information available.

Viscosity, dynamic
No information available.

Explosive properties
No information available.

SECTION 10. Stability and reactivity
Reactivity
See below

Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents, Strong acids, strong reducing agents, Bases

Conditions to avoid
no information available

Incompatible materials
no information available

Hazardous decomposition products
no information available

SECTION 11. Toxicological information
Information on toxicological effects
Likely route of exposure
Eye contact, Skin contact, Ingestion

Skin irritation
Causes skin irritation.

Eye irritation
Causes serious eye irritation.

Specific target organ systemic toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

OSHA: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information:
Quantitative data on the toxicity of this product are not available.

Further data:
Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity
No information available.

Persistence and degradability
No information available.

Bioaccumulative potential
*Partition coefficient: n-octanol/water*
log Pow: 1.20  
(calculated)  
Bioaccumulation is not expected (log Pow <1). (Lit.)

Mobility in soil
No information available.

Other adverse effects
*Additional ecological information*
We have no quantitative data concerning the ecological effects of this product.

Further information on ecology
Discharge into the environment must be avoided.

SECTION 13. Disposal considerations
The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.
SECTION 14. Transport information

Land transport (DOT)
Not classified as dangerous in the meaning of transport regulations.

Air transport (IATA)
Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)
Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

Canada

WHMIS Classification
D2B Toxic Material Causing Other Toxic Effects
Skin irritant, Eye irritant
This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

Notification status
TSCA: Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes.
Ingredients
Benzoylformic acid

DSL: This product contains one or several components that are not on the Canadian DSL nor NDSL.
Ingredients
Benzoylformic acid

SECTION 16. Other information

Training advice
Provide adequate information, instruction and training for operators.

Full text of H-Statements referred to under sections 2 and 3.
H315 Causes skin irritation.
H319 Causes serious eye irritation.

Key or legend to abbreviations and acronyms used in the safety data sheet
Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Date of issue: 03/16/2013
The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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