



BENZOIC ACID (CARBOXYL-13C, 99%)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 27/01/2011

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Version: 5.0

CLM-657

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form : Substance
Substance name : BENZOIC ACID (CARBOXYL-13C, 99%)
EC-No. : 200-618-2 (Unlabeled)
CAS-No. : 3880-99-7
Product code : CLM-657
Formula : C6H5*COOH

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

1.2.1. Relevant identified uses

Main use category : Professional use
Industrial/Professional use spec : For professional use only

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810
USA

USA: 1-800-322-1174 Int: 1-978-749-8000
cilsales@isotope.com www.isotope.com

Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)
International: 1-703-741-5970 (24 hours)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute Tox. 4 (Oral) H302
Eye Dam. 1 H318
STOT SE 3 H335

Full text of hazard classes and H-statements : see section 16

Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Xn; R22
Xi; R41
Xi; R37

Full text of R-phrases: see section 16

GHS-US classification

Acute Tox. 4 (Oral) H302
Eye Dam. 1 H318
STOT SE 3 H335

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

No additional information available

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2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



Signal word (CLP) :

Danger

Hazard statements (CLP) :

H302 - Harmful if swallowed
H318 - Causes serious eye damage
H335 - May cause respiratory irritation

Precautionary statements (CLP) :

P261 - Avoid breathing dust, mist.
P264 - Wash Both hands thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear eye protection, face protection, protective clothing, protective gloves.
P301+P312 - IF SWALLOWED: Call a doctor if you feel unwell.
P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H302 - Harmful if swallowed
H318 - Causes serious eye damage
H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P261 - Avoid breathing dust, mist.
P264 - Wash Both hands thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear eye protection, face protection, protective gloves, protective clothing.
P301+P312 - If swallowed: Call a poison center or doctor if you feel unwell
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310 - Immediately call a poison center or doctor
P312 - Call a poison center or doctor if you feel unwell
P330 - Rinse mouth.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to Comply with applicable regulations

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
BENZOIC ACID (CARBOXYL-13C, 99%)	(CAS-No.) 3880-99-7 (EC-No.) 200-618-2 (Unlabeled)	100	Xn; R22 Xi; R41 Xi; R37

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
BENZOIC ACID (CARBOXYL-13C, 99%)	(CAS-No.) 3880-99-7 (EC-No.) 200-618-2 (Unlabeled)	100	Acute Tox. 4 (Oral), H302 Eye Dam. 1, H318 STOT SE 3, H335

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Full text of R- and H- phrases: see section 16

Name	Product identifier	%	GHS-US classification
BENZOIC ACID (CARBOXYL-13C, 99%) (Main constituent)	(CAS-No.) 3880-99-7	100	Acute Tox. 4 (Oral), H302 Eye Dam. 1, H318 STOT SE 3, H335

Full text of H-phrases: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

- First-aid measures general : Move out of dangerous area. Consult a physician and show this safety data sheet.
- First-aid measures after inhalation : If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
- First-aid measures after skin contact : Wash with soap and plenty of water. Consult a physician.
- First-aid measures after eye contact : Flush eye with water for 15 minutes. Get medical attention.
- First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2. Most important symptoms and effects, both acute and delayed

- Symptoms/effects after inhalation : May be harmful if inhaled. May cause respiratory tract irritation.
- Symptoms/effects after skin contact : May be harmful if absorbed through skin. May cause skin irritation.
- Symptoms/effects after eye contact : Causes serious eye damage.
- Symptoms/effects after ingestion : Harmful if swallowed.

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

- Suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

5.2. Special hazards arising from the substance or mixture

No additional information available

5.3. Advice for firefighters

- Firefighting instructions : Wear self contained breathing apparatus for fire fighting if necessary.
- Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

- Emergency procedures : Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3. Methods and material for containment and cleaning up

- For containment : Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

- Additional hazards when processed : Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.
- Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Keep container tightly closed in a cool, dry and well-ventilated place.
Storage conditions : Store at room temperature away from light and moisture.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)	
DNEL/DMEL (Workers)	
Long-term - systemic effects, dermal	62.5 mg/kg bodyweight/day
Long-term - systemic effects, inhalation	3 mg/m ³
Long-term - local effects, inhalation	0.1 mg/m ³
PNEC (Water)	
PNEC aqua (marine water)	0.034 mg/l
PNEC (Sediment)	
PNEC sediment (freshwater)	1.75 mg/kg dwt
PNEC sediment (marine water)	0.175 mg/kg dwt
PNEC (Soil)	
PNEC soil	0.151 mg/kg dwt
PNEC (STP)	
PNEC sewage treatment plant	100 mg/l

Additional information : Aquatic intermittent release- 0.331 mg/l

8.2. Exposure controls

Personal protective equipment : Safety glasses. Gloves. Protective clothing. Self-contained breathing apparatus.



Hand protection : Wear suitable protective clothing and gloves.
Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.
Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.
Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Solid
Appearance : Crystalline.
Molecular mass : 123.11 g/mol (Labeled)
Color : White.
Odor : No data available
Odor threshold : No data available
pH : 2.5 - 3.5 at 20 °C (68 °F)
Relative evaporation rate (butyl acetate=1) : No data available
Melting point : 121 - 125 °C (250 - 257 °F) - lit.
Freezing point : No data available
Boiling point : 249 °C (480 °F) - lit.
Flash point : 121 °C (250 °F) - closed cup
Auto-ignition temperature : 572 °C (1,062 °F)
Decomposition temperature : No data available
Flammability (solid, gas) : No data available
Vapor pressure : 13 hPa (10 mmHg) at 132 °C (270 °F).
Relative vapor density at 20 °C : 4.22 - (Air = 1.0)
Relative density : 1.32 g/cm³ at 20 °C (68 °F)
Solubility : Water: 2.9 g/l at 25 °C (77 °F)
Log Pow : 1.88

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Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosion limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Not available.

10.5. Incompatible materials

Strong oxidizing agents, Strong bases, Strong reducing agents.

10.6. Hazardous decomposition products

formed under fire conditions: Carbon oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed.

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)	
LD50 oral rat	2360 mg/kg - female. (OECD Test Guideline 401); Remarks: Behavioral:Somnolence (general depressed activity). Cyanosis
LD50 dermal rabbit	> 2000 mg/kg
LC50 inhalation rat (mg/l)	> 12.2 mg/l - 4 h
ATE CLP (oral)	1700.000 mg/kg body weight
ATE CLP (dermal)	10000.000 mg/kg body weight

Skin corrosion/irritation	: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) pH: 2.5 - 3.5 at 20 °C (68 °F)
Serious eye damage/irritation	: Eyes - Rabbit Result: Corrosive. (Directive 67/548/EEC, Annex V, B.5.) Eyes - rabbit - Severe eye irritation pH: 2.5 - 3.5 at 20 °C (68 °F)
Respiratory or skin sensitization	: Maximisation Test - Guinea pig. Result: Does not cause skin sensitisation. (OECD Test Guideline 406) No data available
Germ cell mutagenicity	: Ames test. S. typhimurium result: negative
Carcinogenicity	: Not classified
Reproductive toxicity	: Not available
Specific target organ toxicity – single exposure	: May cause respiratory irritation. No data available
Specific target organ toxicity – repeated exposure	: Inhalation - Causes damage to organs through prolonged or repeated exposure. - Lungs No data available
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation.
Symptoms/effects after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact	: Causes serious eye damage.
Symptoms/effects after ingestion	: Harmful if swallowed.

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SECTION 12: Ecological information

12.1. Toxicity

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)

LC50 fish 1	44.6 mg/l - Lepomis macrochirus - 96 h
EC50 Daphnia 1	860 mg/l Immobilization EC50 - Daphnia magna (Water flea) - 48 h
ErC50 (algae)	> 33.1 mg/l static test EC50 - Pseudokirchneriella subcapitata -72 h. (OECD Test Guideline 201)

12.2. Persistence and degradability

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)

Persistence and degradability	Expected to be biodegradable.
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12.3. Bioaccumulative potential

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)

Bioconcentration factor (BCF REACH)	5.3
Log Pow	1.88
Bioaccumulative potential	Bioaccumulation: Leuciscus idus (Golden orfe) - 3 d . - 50 µg/l.

12.4. Mobility in soil

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)

Ecology - soil	Not available.
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12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : An environmental hazard cannot be excluded in the event of an unprofessional handling or disposal. Harmful to aquatic life.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste)	: Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.
Product/Packaging disposal recommendations	: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
Ecology - waste materials	: Dispose of as unused product.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

14.1. UN number

UN-No.(DOT)	: 3077
DOT NA no.	UN3077

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Environmentally hazardous substances, solid, n.o.s.
Class (DOT)	: 9 - Class 9 - Miscellaneous hazardous material 49 CFR 173.140
Hazard labels (DOT)	: 9 - Class 9 (Miscellaneous dangerous materials)



DOT Symbols	: G - Identifies PSN requiring a technical name
Packing group (DOT)	: III - Minor Danger

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DOT Special Provisions (49 CFR 172.102)	: 8 - A hazardous substance that is not a hazardous waste may be shipped under the shipping description "Other regulated substances, liquid or solid, n.o.s.", as appropriate. In addition, for solid materials, special provision B54 applies. 146 - This description may be used for a material that poses a hazard to the environment but does not meet the definition for a hazardous waste or a hazardous substance, as defined in 171.8 of this subchapter, or any hazard class as defined in Part 173 of this subchapter, if it is designated as environmentally hazardous by the Competent Authority of the country of origin, transit or destination. 335 - Mixtures of solids that are not subject to this subchapter and environmentally hazardous liquids or solids may be classified as "Environmentally hazardous substances, solid, n.o.s.," UN3077 and may be transported under this entry, provided there is no free liquid visible at the time the material is loaded or at the time the packaging or transport unit is closed. Each transport unit must be leak-proof when used as bulk packaging. A112 - Notwithstanding the quantity limits shown in Column (9A) and (9B) for this entry, the following IBCs are authorized for transportation aboard passenger and cargo-only aircraft. Each IBC may not exceed a maximum net quantity of 1,000 kg: a. Metal: 11A, 11B, 11N, 21A, 21B and 21N b. Rigid plastics: 11H1, 11H2, 21H1 and 21H2 c. Composite with plastic inner receptacle: 11HZ1, 11HZ2, 21HZ1 and 21HZ2 d. Fiberboard: 11G e. Wooden: 11C, 11D and 11F (with inner liners) f. Flexible: 13H2, 13H3, 13H4, 13H5, 13L2, 13L3, 13L4, 13M1 and 13M2 (flexible IBCs must be sift-proof and water resistant or must be fitted with a sift-proof and water resistant liner). B54 - Open-top, sift-proof rail cars are also authorized. IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2). IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner. N20 - A 5M1 multi-wall paper bag is authorized if transported in a closed transport vehicle. T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2) TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 155
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 213
DOT Packaging Bulk (49 CFR 173.xxx)	: 240
DOT RQ	: 5000 lbs
Marine pollutant	: No

14.3. Additional information

Other information	: No supplementary information available.
Special transport precautions	: IMDG/IATA - Not dangerous goods.

Overland transport

Packing group (ADR)	: III
Class (ADR)	: 9 - Miscellaneous dangerous substances and articles
Hazard identification number (Kemler No.)	: 90
Classification code (ADR)	: M7
Hazard labels (ADR)	: 9 - Miscellaneous dangerous substances and articles



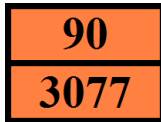
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Orange plates

:



Tunnel restriction code (ADR)

: E

Limited quantities (ADR)

5kg

EAC

: Z2

Excepted quantities (ADR)

: E1

Transport by sea

DOT Vessel Stowage Location

: A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

MFAG-No

: 171

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)

: No limit

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)

: No limit

Civil Aeronautics Law

: Miscellaneous dangerous substances & articles

14.4. Environmental hazards

Other information

: No supplementary information available.

14.5. Special precautions for user

Special transport precautions

: IMDG/IATA - Not dangerous goods.

14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)

SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard
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15.2. International regulations

CANADA

BENZOIC ACID (CARBOXYL-13C, 99%) (3880-99-7)

Listed on the Canadian DSL (Domestic Substances List)

15.2.1. National regulations

No additional information available

15.3. US State regulations

BENZOIC ACID (CARBOXYL-13C, 99%)(3880-99-7)

U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	RTK - U.S. - Massachusetts - Right To Know List RTK - U.S. - Pennsylvania - RTK (Right to Know) List RTK - U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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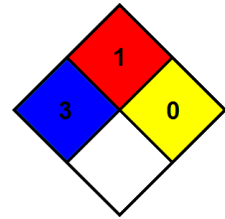
SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of R-, H- and EUH-phrases:

Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Eye Dam. 1	Serious eye damage/eye irritation Category 1
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H302	Harmful if swallowed
H318	Causes serious eye damage
H335	May cause respiratory irritation
R22	Harmful if swallowed
R37	Irritating to respiratory system
R41	Risk of serious damage to eyes
Xi	Irritant
Xn	Harmful

NFPA health hazard : 3 - Materials that, under emergency conditions, can cause serious or permanent injury.
NFPA fire hazard : 1 - Materials that must be preheated before ignition can occur.
NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
Flammability : 1 Slight Hazard
Physical : 0 Minimal Hazard

CIL Substance SDS

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product