



2,4-PENTANEDIONE (13C5, 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: 10/01/2011

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Supersedes: 10/01/2011

Version: 2.0

CLM-6756

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

1.1. Product identifier

Product form : Substance
Substance name : 2,4-PENTANEDIONE (13C5, 99%)
EC Index-No. : 606-029-00-0 (Unlabeled)
EC-No. : 204-634-0 (Unlabeled)
CAS-No. : 123-54-6 (Unlabeled)
Product code : CLM-6756
Formula : *CH3*CO*CH2*CO*CH3

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]

Flam. Liq. 3 H226
Acute Tox. 3 (Oral) H301
Acute Tox. 3 (Dermal) H311
Eye Dam. 1 H318

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

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

R10
T; R24/25
Xi; R41

Full text of R-phrases: see section 16

GHS-US classification

Flam. Liq. 3 H226
Acute Tox. 3 (Oral) H301
Acute Tox. 3 (Dermal) H311
Eye Dam. 1 H318

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) :

H226 - Flammable liquid and vapor
H301+H311 - Toxic if swallowed or in contact with skin
H318 - Causes serious eye damage

Precautionary statements (CLP) :

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 - Keep container tightly closed.
P240 - Ground/bond container and receiving equipment.
P241 - Use explosion-proof electrical/ventilating/lighting equipment
P264 - Wash hands, forearms and face thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor.

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H226 - Flammable liquid and vapor
H301+H311 - Toxic if swallowed or in contact with skin
H318 - Causes serious eye damage

Precautionary statements (GHS-US) :

P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233 - Keep container tightly closed.
P240 - Ground/Bond container and receiving equipment
P241 - Use explosion-proof electrical/ventilating/lighting equipment
P242 - Use only non-sparking tools.
P243 - Take precautionary measures against static discharge.
P264 - Wash hands, forearms and face thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P301+P310 - If swallowed: Immediately call a poison center or doctor
P302+P352 - If on skin: Wash with plenty of water
P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
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
P321 - Specific treatment (see supplemental first aid instruction on this label)
P322 - Specific treatment (see supplemental first aid instruction on this label)
P330 - Rinse mouth.
P361+P364 - Take off immediately all contaminated clothing and wash it before reuse.
P370+P378 - In case of fire: Use media other than water to extinguish.
P403+P235 - Store in a well-ventilated place. Keep cool.
P405 - Store locked up.
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

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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

Name	Product identifier	%	Classification according to Directive 67/548/EEC
2,4-PENTANEDIONE (13C5, 99%)	(CAS-No.) 123-54-6 (Unlabeled) (EC-No.) 204-634-0 (Unlabeled) (EC Index-No.) 606-029-00-0 (Unlabeled)	100	R10 T; R24/25 Xi; R41

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
2,4-PENTANEDIONE (13C5, 99%)	(CAS-No.) 123-54-6 (Unlabeled) (EC-No.) 204-634-0 (Unlabeled) (EC Index-No.) 606-029-00-0 (Unlabeled)	100	Flam. Liq. 3, H226 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Eye Dam. 1, H318

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

Name	Product identifier	%	GHS-US classification
2,4-PENTANEDIONE (13C5, 99%) (Main constituent)	(CAS-No.) 123-54-6 (Unlabeled)	100	Flam. Liq. 3, H226 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Eye Dam. 1, H318

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	: If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.
First-aid measures after inhalation	: When symptoms occur: go into open air and ventilate suspected area. If not breathing give artificial respiration. Get medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of soap and water. and soap. Get immediate medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

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

Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory irritation.
Symptoms/effects after skin contact	: Toxic in contact with skin.
Symptoms/effects after eye contact	: Causes serious eye damage.
Symptoms/effects after ingestion	: Toxic 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	: For small fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.
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5.2. Special hazards arising from the substance or mixture

Fire hazard	: Flammable liquid and vapor.
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5.3. Advice for firefighters

Firefighting instructions	: Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures	: Avoid breathing vapors, mist, gas. Avoid dust formation.
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6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

For containment : Clean up any spills as soon as possible, using an absorbent material to collect it. Small quantities of liquid spill: take up in non-combustible absorbent material and shovel into container for disposal. For large spills, confine the spill in a dike and charge it with wet sand or earth for subsequent safe disposal.

Methods for cleaning up : This material and its container must be disposed of in a safe way, and as per local legislation.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Provide adequate ventilation to minimize dust and/or vapor concentrations.

Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Store in a well-ventilated place. Keep container tightly closed.

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

No additional information available

8.2. Exposure controls

Appropriate engineering controls : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

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



Materials for protective clothing : Wear suitable protective clothing and gloves.

Hand protection : Wear suitable protective clothing and gloves.

Eye protection : Wear eye protection. Chemical goggles or face shield with safety glasses.

Skin and body protection : Wear suitable protective clothing, gloves and eye/face protection.

Respiratory protection : In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator.

Environmental exposure controls : Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Liquid

Appearance : Liquid

Molecular mass : 105.08 g/mol (Labeled)

Color : Clear

Odor : No data available

Odor threshold : No data available

pH : 6 at 200 g/l at 20 °C (68 °F)

Relative evaporation rate (butyl acetate=1) : No data available

Melting point : -23 °C (- 9 °F) - lit

Freezing point : No data available

Boiling point : 140.4 °C (284.7 °F) - lit

Flash point : 38 °C (100 °F) - closed cup

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Auto-ignition temperature	: 350 °C (662 °F)
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: No data available
Relative vapor density at 20 °C	: 3.46 (Air = 1.0)
Relative density	: No data available
Specific gravity / density	: 0.975 g/cm ³ at 25 °C (77 °F)
Solubility	: Soluble in water.
Log Pow	: 1.9
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	: 1.7 - 11.4 vol %

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Five years after receipt if stored as stated in "Storage" section. Re-QC after 5 years.

10.3. Possibility of hazardous reactions

Vapors may form explosive mixture with air.

10.4. Conditions to avoid

No additional information available

10.5. Incompatible materials

Strong oxidizing agents. Reducing agents. Strong bases. Metals.

10.6. Hazardous decomposition products

Carbon oxides (CO, CO₂).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Toxic if swallowed. Dermal: Toxic in contact with skin.

2,4-PENTANEDIONE (13C5, 99%) (123-54-6 (Unlabeled))	
LD50 oral rat	55 mg/kg
LD50 dermal rabbit	787 mg/kg
ATE CLP (oral)	100.000 mg/kg body weight
ATE CLP (dermal)	300.000 mg/kg body weight

Skin corrosion/irritation	: Not classified pH: 6 at 200 g/l at 20 °C (68 °F)
Serious eye damage/irritation	: Eyes - Rabbit Result: Severe eye irritation pH: 6 at 200 g/l at 20 °C (68 °F)
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Laboratory experiments have shown mutagenic effects.
Carcinogenicity	: Not classified
Reproductive toxicity	: Laboratory experiments have shown teratogenic effects. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.
Specific target organ toxicity – single exposure	: Not classified
Specific target organ toxicity – repeated exposure	: Not classified
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: 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.

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Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory irritation.
Symptoms/effects after skin contact	: Toxic in contact with skin.
Symptoms/effects after eye contact	: Causes serious eye damage.
Symptoms/effects after ingestion	: Toxic if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

2,4-PENTANEDIONE (13C5, 99%) (123-54-6 (Unlabeled))

LC50 fish 1	106 mg/l other fish - 96 h
EC50 Daphnia 1	40 mg/l - Daphnia magna (Water flea) - 24 h

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

2,4-PENTANEDIONE (13C5, 99%) (123-54-6 (Unlabeled))

Log Pow	1.9
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12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

No additional information available

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)	: 2310
DOT NA no.	UN2310

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Pentane-2,4-dione
Class (DOT)	: 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
Hazard labels (DOT)	: 3 - Flammable liquid 6.1 - Poison



Packing group (DOT)	: III - Minor Danger
DOT Special Provisions (49 CFR 172.102)	: B1 - If the material has a flash point at or above 38 C (100 F) and below 93 C (200 F), then the bulk packaging requirements of 173.241 of this subchapter are applicable. If the material has a flash point of less than 38 C (100 F), then the bulk packaging requirements of 173.242 of this subchapter are applicable. IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3) TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = 97 / 1 + a (tr - tf) Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 150

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DOT Packaging Non Bulk (49 CFR 173.xxx) : 203
DOT Packaging Bulk (49 CFR 173.xxx) : 242

14.3. Additional information

Emergency Response Guide (ERG) Number : 131
Other information : No supplementary information available.

Overland transport

Packing group (ADR) : III
Class (ADR) : 3 - Flammable liquid
Hazard identification number (Kemler No.) : 36
Classification code (ADR) : FT1
Hazard labels (ADR) : 3 - Flammable liquids
6.1 - Toxic substances



Orange plates :

Tunnel restriction code (ADR) : D/E
Limited quantities (ADR) : 5I
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 : 131

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 60 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 220 L
Civil Aeronautics Law : Flammable liquids

14.4. Environmental hazards

Other information : No supplementary information available.

14.5. Special precautions for user

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

2,4-PENTANEDIONE (13C5, 99%) (123-54-6 (Unlabeled))	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Delayed (chronic) health hazard Fire hazard Immediate (acute) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313.

15.2. International regulations

CANADA

2,4-PENTANEDIONE (13C5, 99%) (123-54-6 (Unlabeled))
Listed on the Canadian DSL (Domestic Substances List)

15.2.1. National regulations

No additional information available

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15.3. US State regulations

2,4-PENTANEDIONE (13C5, 99%)(123-54-6 (Unlabeled))	
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	U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Massachusetts - Right To Know List

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.

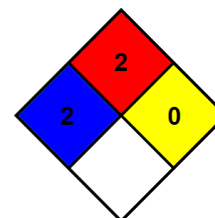
Full text of R-, H- and EUH-phrases:

Acute Tox. 3 (Dermal)	Acute toxicity (dermal) Category 3
Acute Tox. 3 (Oral)	Acute toxicity (oral) Category 3
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Flam. Liq. 3	Flammable liquids Category 3
H226	Flammable liquid and vapor
H301	Toxic if swallowed
H311	Toxic in contact with skin
H318	Causes serious eye damage
R10	Flammable
R24/25	Toxic in contact with skin and if swallowed
R41	Risk of serious damage to eyes
T	Toxic
Xi	Irritant

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 2 Moderate 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