



MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 03/11/2013

Version 1.0

SECTION 1. Identification

Product identifier

Product number 800105
Product name 2,5-Hexanedione for synthesis

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

Identified uses Chemical for synthesis

Details of the supplier of the safety data sheet

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United States of America | SDS Phone Support: +1-978-715-1335 |
General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to
4:00 PM Eastern Time (GMT-5)

e-mail: mm_sds@merckgroup.com

Emergency telephone 800-424-9300 CHEMTREC (USA)
+1-703-527-3887 CHEMTREC (International)
24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

Acute toxicity, Category 3, Inhalation, H331
Acute toxicity, Category 4, Oral, H302
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
Danger

Hazard Statements

H302 Harmful if swallowed.
H319 Causes serious eye irritation.

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H331 Toxic if inhaled.

Precautionary Statements

P262 Do not get in eyes, on skin, or on clothing.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$\text{CH}_3\text{COCH}_2\text{CH}_2\text{COCH}_3$	$\text{C}_6\text{H}_{10}\text{O}_2$ (Hill)
CAS-No.	110-13-4	
Molar mass	114.14 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

hexane-2,5-dione (>= 90 % - <= 100 %)

110-13-4

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

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. Immediately 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, Dermatitis

Drying-out effect resulting in rough and chapped skin.

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Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

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

Forms explosive mixtures with air on intense heating.

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.

Suppress (knock down) gases/vapors/mists with a water spray jet.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. 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 with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Work under hood. Do not inhale substance/mixture.

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

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

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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. Work under hood. Do not inhale substance/mixture.

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.

Respiratory protection

required when vapors/aerosols 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

Physical state	liquid
Color	colorless
Odor	pleasant
Odor Threshold	No information available.
pH	6.1 at 10 g/l 68 °F (20 °C)
Melting point	-5.4 °C
Boiling point/boiling range	378.0 °F (192.2 °C)
Flash point	174 °F (79 °C) Method: c.c.
Evaporation rate	No information available.

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Flammability (solid, gas)	No information available.
Lower explosion limit	1.5 %(V)
Upper explosion limit	No information available.
Vapor pressure	0.6 hPa at 68 °F (20 °C) 2.6 hPa at 122 °F (50 °C)
Relative vapor density	3.94
Relative density	0.974 g/cm ³ at 68 °F (20 °C)
Water solubility	at 68 °F (20 °C) soluble
Partition coefficient: n-octanol/water	log Pow: -0.27 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	1.43 mPa.s at 77 °F (25 °C)
Explosive properties	No information available.
Ignition temperature	752 °F (400 °C)

SECTION 10. Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Conditions to avoid

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

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Incompatible materials

no information available

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Acute oral toxicity

LD50 rat: 1,600 mg/kg (RTECS)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

absorption

Acute inhalation toxicity

Symptoms: mucosal irritations

absorption

Skin irritation

After long-term exposure to the chemical: Drying-out effect resulting in rough and chapped skin.
Dermatitis

Eye irritation

rabbit

Result: Eye irritation
(RTECS)

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.

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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

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: -0.27

(experimental)

(Lit.) Bioaccumulation is not expected (log Pow <1).

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.

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SECTION 15. Regulatory information

United States of America

OSHA Hazards

Combustible Liquid

Harmful if swallowed.

Eye irritant

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard

Acute Health Hazard

SARA 313

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

DEA List I

Not listed

DEA List II

Not listed

Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know

Ingredients

hexane-2,5-dione

New Jersey Right To Know

Ingredients

hexane-2,5-dione

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Notification status

TSCA: On TSCA Inventory

DSL: This product contains one or several components listed in the Canadian NDSL.
Ingredients
hexane-2,5-dione

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.

H302 Harmful if swallowed.
H319 Causes serious eye irritation.
H331 Toxic if inhaled.

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:03/11/2013

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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