



# MATERIAL SAFETY DATA SHEET

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

Revision Date 08/23/2013

Version 1.1

## SECTION 1. Identification

### Product identifier

Product number 803528  
Product name Diacetyl 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

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

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

Flammable liquid, Category 2, H225  
Acute toxicity, Category 4, Oral, H302  
Acute toxicity, Category 4, Inhalation, H332  
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

Danger

#### Hazard Statements

H225 Highly flammable liquid and vapor.  
H302 + H332 Harmful if swallowed or if inhaled.  
H315 Causes skin irritation.

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H319 Causes serious eye irritation.

### *Precautionary Statements*

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P233 Keep container tightly closed.

P240 Ground/bond container and receiving equipment.

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.

P403 + P235 Store in a well-ventilated place. Keep cool.

### **OSHA Hazards**

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

### **Other hazards**

None known.

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## **SECTION 3. Composition/information on ingredients**

Formula	CH <sub>3</sub> COCOCH <sub>3</sub>	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> (Hill)
CAS-No.	431-03-8	
Molar mass	86.09 g/mol	

### **Hazardous ingredients**

*Chemical Name (Concentration)*

CAS-No.

*butanedione (>= 90 % - <= 100 % )*

431-03-8

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## **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. 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, Nausea, Headache

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The following applies to ketones in general: when vapors/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

### Indication of any immediate medical attention and special treatment needed

No information available.

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## SECTION 5. Fire-fighting measures

### Extinguishing media

*Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), 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.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

Pay attention to flashback.

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*

Cool closed containers exposed to fire with water spray. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## 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. Keep away from heat and sources of ignition. 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. Risk of explosion.

### 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.

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### SECTION 7. Handling and storage

#### Precautions for safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols.

Observe label precautions.

#### *Advice on protection against fire and explosion*

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### Conditions for safe storage, including any incompatibilities

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place.

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.

#### *Other protective equipment:*

Flame retardant antistatic protective clothing

#### *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.

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### SECTION 9. Physical and chemical properties

Physical state liquid

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Color	yellow
Odor	sweet
Odor Threshold	No information available.
pH	No information available.
Melting point	-2 °C
Boiling point/boiling range	192 - 194 °F (89 - 90 °C) at 1,013 hPa
Flash point	41 °F (5 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	2.4 %(V)
Upper explosion limit	13.0 %(V)
Vapor pressure	52 hPa at 68 °F (20 °C)  229 hPa at 122 °F (50 °C)
Relative vapor density	No information available.
Relative density	0.99 g/cm <sup>3</sup> at 68 °F (20 °C)
Water solubility	200 g/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: -1.34 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	> 230 °F (> 110 °C)
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Ignition temperature	689 °F (365 °C)

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**SECTION 10. Stability and reactivity**

**Reactivity**

Vapors may form explosive mixture with air.

**Chemical stability**

heat-sensitive

**Possibility of hazardous reactions**

Violent reactions possible with:

alkalines, Acids

Risk of ignition or formation of inflammable gases or vapors with:

strong oxidizing agents

**Conditions to avoid**

Warming.

**Incompatible materials**

various plastics

**Hazardous decomposition products**

no information available

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**SECTION 11. Toxicological information**

**Information on toxicological effects**

*Likely route of exposure*

Inhalation, Eye contact, Skin contact

*Acute oral toxicity*

LD50 rat: 1,580 mg/kg (RTECS)

absorption

*Acute inhalation toxicity*

LC50 rat: 2.25 - 5.2 mg/l; 4 h (External MSDS)

absorption

Symptoms: Possible damages:, Irritation symptoms in the respiratory tract.

*Acute dermal toxicity*

LD50 rabbit: > 5,000 mg/kg  
(RTECS)

*Skin irritation*

rabbit

Result: Irritations  
(External MSDS)

Causes skin irritation.

*Eye irritation*

Causes serious eye irritation.

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### *Sensitization*

Sensitization test: guinea pig

Result: negative

(External MSDS)

### *Genotoxicity in vivo*

Mutagenicity (mammal cell test): micronucleus.

Result: negative

(National Toxicology Program)

### *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**

After absorption of toxic quantities:

Headache, Nausea

The following applies to ketones in general: when vapors/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract. Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12. Ecological information**

### **Ecotoxicity**

#### *Toxicity to fish*

LC50 *Leuciscus idus* (Golden orfe): 46 - 100 mg/l; 96 h (External MSDS)

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*Toxicity to bacteria*

EC50 *Pseudomonas putida*: 42 mg/l; 17 h (Hommel)

**Persistence and degradability**

*Biodegradability*

Readily biodegradable.

**Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: -1.34

(experimental)

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

**Mobility in soil**

No information available.

*Additional ecological information*

Discharge into the environment must be avoided.

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**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.

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**SECTION 14. Transport information**

**Land transport (DOT)**

UN number	UN 2346
Proper shipping name	BUTANEDIONE
Class	3
Packing group	II
Environmentally hazardous	--

**Air transport (IATA)**

UN number	UN 2346
Proper shipping name	BUTANEDIONE
Class	3
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

**Sea transport (IMDG)**

UN number	UN 2346
Proper shipping name	BUTANEDIONE
Class	3
Packing group	II
Environmentally hazardous	--



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**Special precautions for user** yes  
EmS F-E S-D

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**SECTION 15. Regulatory information**

**United States of America**

**OSHA Hazards**

Flammable Liquid  
Toxic by inhalation.  
Harmful if swallowed.  
Skin irritant  
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

**US State Regulations**

**Massachusetts Right To Know**

*Ingredients*  
butanedione

**Pennsylvania Right To Know**

*Ingredients*  
butanedione

**New Jersey Right To Know**

*Ingredients*  
butanedione

**California Prop 65 Components**

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This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

## Notification status

TSCA: All components of the product are listed in the TSCA-inventory.

DSL: All components of this product are on the Canadian DSL.

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## 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.

H225 Highly flammable liquid and vapor.  
H302 Harmful if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H332 Harmful 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](http://www.wikipedia.org).

Revision Date 08/23/2013

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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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