SAFETY DATA SHEET

Version 8.3
Revision Date 09/10/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Acetylacetone

Product Number : A3511
Brand : Sigma
Index-No. : 606-029-00-0
CAS-No. : 123-54-6

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Short-term (acute) aquatic hazard (Category 3), H402

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

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H311 + H331	Toxic in contact with skin or if inhaled.
H402	Harmful to aquatic life.

Precautionary statement(s)

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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	:	2,4-Pentanedione
Formula	:	CH3COCH2COCH3
Molecular weight	:	100.12 g/mol
CAS-No.	:	123-54-6
EC-No.	:	204-634-0
Index-No.	:	606-029-00-0

Component	Classification	Concentration
Acetylacetone		
	Flam. Liq. 3; Acute Tox. 4; Acute Tox. 3; Aquatic Acute 3; H226, H302,	<= 100 %

	H331, H311, H402	

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Consult a physician. Show this material safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Do NOT induce vomiting. 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
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Dry powder Dry sand

Unsuitable extinguishing media
Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.
For personal protection see section 8.

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 materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion
Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

Hygiene measures
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage class
Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Acetylacetone	123-54-6	TWA	25 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		

8.2 Exposure controls

Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Splash contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 120 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and

components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Color: colorless
b)	Odor	malodorous
c)	Odor Threshold	No data available
d)	pH	6 at 200 g/l at 20 °C (68 °F)
e)	Melting point/freezing point	Melting point/range: ca.-47.5 - -17.6 °C (ca.-53.5 - 0.3 °F) at 1,013 hPa - OECD Test Guideline 102
f)	Initial boiling point and boiling range	ca.139.5 °C ca.283.1 °F at 1,013 hPa - OECD Test Guideline 103
g)	Flash point	35 °C (95 °F) - Non-equilibrium method - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 11.4 %(V) Lower explosion limit: 2.4 %(V)
k)	Vapor pressure	ca.7.9 hPa at ca.20 °C (ca.68 °F) - OECD Test Guideline 104 ca.40.4 hPa at ca.50 °C(ca.122 °F) - OECD Test Guideline 104
l)	Vapor density	3.5 - (Air = 1.0)
m)	Density	0.97 g/cm3 at 20 °C (68 °F) - OECD Test Guideline 109
	Relative density	No data available
n)	Water solubility	ca.153.8 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o)	Partition coefficient: n-octanol/water	log Pow: ca.0.68 at 40 °C (104 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.
p)	Autoignition temperature	No data available
q)	Decomposition temperature	Distillable in an undecomposed state at normal pressure.
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information

Surface tension	72 mN/m at 1g/l at 20 °C (68 °F) - OECD Test Guideline 115
Relative vapor	3.5 - (Air = 1.0)

density

SECTION 10: Stability and reactivity

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - female - 570 mg/kg
Remarks: (ECHA)
LC50 Inhalation - Rat - male and female - 4 h - 5.0305 mg/l
(OECD Test Guideline 403)
Symptoms: mucosal irritations, Cough
LD50 Dermal - Rabbit - female - 790 mg/kg
Remarks: (ECHA)
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
Remarks: (ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: slight irritation
Remarks: (ECHA)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity
Laboratory experiments have shown mutagenic effects.
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Test system: Chinese hamster ovary cells
Metabolic activation: without metabolic activation

Method: OECD Test Guideline 473
Result: positive
Test Type: sister chromatid exchange assay
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 479
Result: positive
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: inhalation (vapor)
Method: US-EPA
Result: negative

Test Type: comet assay
Species: Rat
Cell type: Liver cells
Application Route: Oral

Result: negative
Remarks: (ECHA)

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.

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.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
Ingestion of excessive amounts by pregnant animals resulted in maternal and fetal toxicity.
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

Repeated dose toxicity - Rabbit - male and female - Dermal - 9 Days - NOAEL (No observed adverse effect level) - 244 mg/kg - LOAEL (Lowest observed adverse effect level) - 975 mg/kg
Remarks: (ECHA)

Inhalation may provoke the following symptoms:, Dizziness, Suffocation
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Systemic effects:

Dizziness
Headache
Shortness of breath
respiratory arrest
Unconsciousness

Damage to:

Liver
Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 104 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 25.9 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 83.22 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 107.6 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d

Result: 83 - 100 % - Readily biodegradable.
(OECD Test Guideline 301C)

Ratio BOD/ThBOD 5.6 %
Remarks: (Lit.)

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.
Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

DOT (US)
UN number: 2310 Class: 3 (6.1) Packing group: III
Proper shipping name: Pentane-2,4-dione
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 2310 Class: 3 (6.1) Packing group: III EMS-No: F-E, S-D
Proper shipping name: PENTANE-2,4-DIONE

IATA
UN number: 2310 Class: 3 (6.1) Packing group: III
Proper shipping name: Pentane-2,4-dione

SECTION 15: Regulatory information

SARA 302 Components

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

SARA 313 Components
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 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Acetylacetone	123-54-6	1993-04-24

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Acetylacetone	123-54-6	1993-04-24

	CAS-No.	Revision Date
Acetylacetone	123-54-6	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Acetylacetone	123-54-6	1993-04-24

SECTION 16: Other information

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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