

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : 3-Pentanone

Product Number : 345121
Brand : Sigma-Aldrich
Index-No. : 606-006-00-5

CAS-No. : 96-22-0

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
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225

Eye irritation (Category 2A), H319

Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

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)

H225

Highly flammable liquid and vapour.

H319

Causes serious eye irritation.

H335

May cause respiratory irritation.

H336

May cause drowsiness or dizziness.

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/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	: Diethyl ketone
Formula	: C ₅ H ₁₀ O
Molecular weight	: 86.13 g/mol
CAS-No.	: 96-22-0
EC-No.	: 202-490-3
Index-No.	: 606-006-00-5

Hazardous components

Component	Classification	Concentration
Diethyl ketone	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H335, H336	<= 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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

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 data available
- 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.

6. ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures**
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours 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.
- 6.3 Methods and materials for containment and cleaning up**
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).
- 6.4 Reference to other sections**
For disposal see section 13.

7. HANDLING AND STORAGE

- 7.1 Precautions for safe handling**
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.
- 7.2 Conditions for safe storage, including any incompatibilities**
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.
- 7.3 Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Diethyl ketone	96-22-0	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Upper Respiratory Tract irritation		
		TWA	200.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment		

		Upper Respiratory Tract irritation		
		STEL	300 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		STEL	300.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		TWA	200.000000 ppm 705.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		STEL	300 ppm 1,057 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		PEL	200 ppm 705 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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.

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 30 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

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 CE 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.

Body Protection

Impervious clothing, 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Colour: colourless
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	6.2 at 50 g/l at 20 °C (68 °F)
e) Melting point/freezing point	Melting point/range: -42 °C (-44 °F) - lit.
f) Initial boiling point and boiling range	101.5 °C (214.7 °F) - lit.
g) Flash point	7 °C (45 °F) - 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: 7.7 %(V) Lower explosion limit: 1.6 %(V)
k) Vapour pressure	37.5 hPa (28.1 mmHg) at 20 °C (68 °F)
l) Vapour density	2.97 - (Air = 1.0)
m) Relative density	0.813 g/cm ³ at 25 °C (77 °F)
n) Water solubility	50 g/l at 20 °C (68 °F)
o) Partition coefficient: n-octanol/water	log Pow: 0.85
p) Auto-ignition temperature	455 °C (851 °F)
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

Surface tension	25.33 mN/m at 15 °C (59 °F)
Relative vapour density	2.97 - (Air = 1.0)

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

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Oxidizing agents, Strong bases

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 2,900 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male - 4 h - 28.5 mg/l
(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male - 16,200 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

(OECD Test Guideline 405)

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

Chromosome aberration test in vitro

Saccharomyces cerevisiae

Result: negative

OECD Test Guideline 474

Chinese hamster - male and female

Result: negative

Carcinogenicity

IARC: No component 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 component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

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

Additional Information

Repeated dose toxicity Rat - female - Oral - 120 d - NOAEL : 1,860 mg/kg

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,540 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - > 500 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.)
Toxicity to algae	static test EC50 - Desmodesmus subspicatus (Scenedesmus subspicatus) - > 500 mg/l - 72 h

12.2 Persistence and degradability

Biodegradability	Zahn-Wellens Test - Exposure time 13 d Result: 90 - 100 % - Readily biodegradable (OECD Test Guideline 302B)
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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

No data available

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

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

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

UN number: 1156 Class: 3 Packing group: II
Proper shipping name: Diethyl ketone
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 1156 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: DIETHYL KETONE

IATA

UN number: 1156 Class: 3 Packing group: II
Proper shipping name: Diethyl ketone

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

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Diethyl ketone	96-22-0	1994-04-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Diethyl ketone	96-22-0	1994-04-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Diethyl ketone	96-22-0	1994-04-01

California Prop. 65 Components

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

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
STOT SE	Specific target organ toxicity - single exposure

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	3
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	3
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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