

SAFETY DATA SHEET

Version 6.4
Revision Date 08/30/2023
Print Date 01/13/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Acetophenone- β,β,β -d₃

Product Number : 318019
Brand : Aldrich
CAS-No. : 17537-31-4

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 4), H227
Acute toxicity, Oral (Category 4), H302
Eye irritation (Category 2A), H319
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

Warning

Aldrich - 318019

Page 1 of 11

Hazard statement(s)	
H227	Combustible liquid.
H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H402	Harmful to aquatic life.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
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.
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 + P235	Store in a well-ventilated place. Keep cool.
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	: Acetophenone-methyl-d3
Formula	: C ₈ D ₃ H ₅ O
Molecular weight	: 123.14 g/mol
CAS-No.	: 17537-31-4
EC-No.	: 687-233-7

Component	Classification	Concentration
Aceto-d3-phenone		
	Flam. Liq. 4; Acute Tox. 4; Eye Irrit. 2A; Aquatic Acute 3; H227, H302, H319, H402	<= 100 %

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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 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. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

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

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

Storage class

Storage class (TRGS 510): 10: Combustible 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
Aceto-d3-phenone	17537-31-4	TWA	10 ppm	USA. ACGIH Threshold Limit Values (TLV)
		TWA	10 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
		PEL	10 ppm 49 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

Splash contact

Material: Latex gloves

Minimum layer thickness: 0.6 mm

Break through time: 30 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A-(P2)

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 19 - 20 °C (66 - 68 °F) - lit.
f) Initial boiling point and boiling range	202 °C 396 °F - lit.
g) Flash point	76.00 °C (168.80 °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: 5.20 %(V) Lower explosion limit: 1.40 %(V)
k) Vapor pressure	1 hPa at 15.00 °C (59.00 °F)
l) Vapor density	No data available
m) Density	1.055 g/mL at 25 °C (77 °F)1.055 g/cm ³ at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	log Pow: 1.600 - Bioaccumulation is not expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Exothermic reaction with:
Strong oxidizing agents
strong alkalis
strong reducing agents

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

No data available
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 815 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: acetophenone

Inhalation: No data available

LD50 Dermal - Rat - male and female - 3,300 mg/kg

(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: acetophenone

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: acetophenone

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

Remarks: (RTECS)

The value is given in analogy to the following substances: acetophenone

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Aldrich - 318019

Page 7 of 11

Test Type: In vitro mammalian cell gene mutation test
 Test system: mouse lymphoma cells
 Metabolic activation: with and without metabolic activation
 Method: OECD Test Guideline 476
 Result: negative
 Remarks: The value is given in analogy to the following substances: acetophenone
 Type: Ames test
 Test system: Salmonella typhimurium
 Metabolic activation: with and without metabolic activation
 Method: OECD Test Guideline 471
 Result: negative
 Remarks: The value is given in analogy to the following substances: acetophenone
 Type: Mutagenicity (mammal cell test): chromosome aberration.
 Test system: Chinese hamster lung cells
 Metabolic activation: Metabolic activation
 Method: OECD Test Guideline 473
 Result: positive
 Remarks: The value is given in analogy to the following substances: acetophenone
 Type: Mutagenicity (mammal cell test): chromosome aberration.
 Test system: Chinese hamster lung cells
 Metabolic activation: without metabolic activation
 Method: OECD Test Guideline 473
 Result: negative
 Remarks: The value is given in analogy to the following substances: acetophenone
 Test Type: Micronucleus test
 Species: Mouse
 Cell type: Red blood cells (erythrocytes)
 Application Route: Intraperitoneal injection
 Method: OECD Test Guideline 474
 Result: negative
 Remarks: The value is given in analogy to the following substances: acetophenone

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

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 - Rat - male and female - Oral - 90 Days - NOAEL (No observed adverse effect level) - 250 mg/kg

Remarks: The value is given in analogy to the following substances: acetophenone

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 162 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: acetophenone
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia magna (Water flea) - 528 mg/l - 48 h Remarks: (ECHA) The value is given in analogy to the following substances: acetophenone
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 86.4 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: acetophenone
Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209) Remarks: The value is given in analogy to the following substances: acetophenone

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 14 d Result: 64.7 % - Readily biodegradable. (OECD Test Guideline 301C) Remarks: The value is given in analogy to the following substances: acetophenone
------------------	---

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

UN number: 3334 Class: 9

Packing group: III

Proper shipping name: Aviation regulated liquid, n.o.s. (Aceto-d3-phenone)

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Aceto-d3-phenone	17537-31-4	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

Aceto-d3-phenone

CAS-No.
17537-31-4

Revision Date
2007-07-01

Pennsylvania Right To Know Components

Aceto-d3-phenone

CAS-No.
17537-31-4

Revision Date
2007-07-01

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact misbranding@sial.com.

Version: 6.4

Revision Date: 08/30/2023

Print Date: 01/13/2024