

Chemical Safety Data Sheet MSDS / SDS

Acetophenone-1,2-13C2

Revision Date:2026-09-13 Revision Number:1

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

Product name : Acetophenone-1,2-13C2
CBnumber : CB9388570
CAS : 190314-15-9
Synonyms : Acetophenone- α,β -13C2;Acetophenone- α,β -13C?

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
Continuerinsing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

Hazard statements

H302 Harmful if swallowed

H318 Causes serious eye damage

SECTION 3: Composition/information on ingredients**Substance**

Product name	: Acetophenone-1,2-13C2
Synonyms	: Acetophenone- α,β -13C2;Acetophenone- α,β -13C?
CAS	: 190314-15-9
MF	: C8H8O
MW	: 122.17

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

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.

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['Acetophenone- a,β-13C2', '190314- 15-9', 'TWA', '10 ppm', 'USA ACGIH Threshold Limit Values (TLV)']
['', 'PEL', '10 ppm49 mg/m3', 'California permissible exposure limits for chemical contaminants (Title 8, Article 107)']	

TWA 10 ppm USA. Workplace Environmental
Exposure Levels (WEEL)

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

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

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	Melting point/range: 19 - 20 °C - lit.
e) Initial boiling point and boiling range	202 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 5.20 %(V) Lower explosion limit: 1.40 %(V)
h) Flash point	76.00 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	log Pow: 1.600 - Bioaccumulation is not expected.
o) Vapor pressure	1 hPa at 15.00 °C
p) Density	1.047 g/cm ³ at 25 °C
Relative density	1.047 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	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 Chemical stability

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

10.2 Possibility of hazardous reactions

Exothermic reaction with:

Strong oxidizing agents strong alkalis strong reducing agents

10.3 Conditions to avoid

Strong heating.

10.4 Incompatible materials

No data available

10.5 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

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

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: acetophenoneTest

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: acetophenoneTest

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

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

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 static test LC50 - Daphnia magna (Water flea) - 528 mg/l - 48 h and other aquatic Remarks: (ECHA) invertebrates 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

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: -

IMDG: -

IATA-DGR: 3334

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA-DGR: Aviation regulated liquid, n.o.s. (Acetophenone-a,β-13C2)

14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA-DGR: 9

14.4 Packaging group

ADR/RID: -

IMDG: -

IATA-DGR: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A22222486

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.