

Safety Data Sheet

Acetophenone-d3

According to Regulation (EC) No. 1907/2006 (REACH)

Classification acc. to 29 CFR 1910.1200

Version number: GHS 1.1

Date of compilation: 2022-09-19

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

1.1 Product identifier

Identification of the substance	Acetophenone-d3
CAS number	17537-31-4
Alternative name(s)	acetophenone-d3, 1-phenylethanone-d3

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

Relevant identified uses	general use
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1.3 Details of the supplier of the safety data sheet

Zeochem AG Joweid 5, CH-8630 Rüti Switzerland	Telephone: +41 44 922 93 93: e-Mail: Info@zeochem.com / info@zeochem.ch: Website: https://www.zeochem.com :
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1.4 Emergency telephone number

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Category	Hazard class and category	Hazard statement
3.10	acute toxicity (oral)	4	Acute Tox. 4	H302
3.3	serious eye damage/eye irritation	2	Eye Irrit. 2	H319
4.1C	hazardous to the aquatic environment - chronic hazard	3	Aquatic Chronic 3	H412

For full text of abbreviations: see SECTION 16.

The most important adverse physicochemical, human health and environmental effects

Spillage and fire water can cause pollution of watercourses.

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2.2 Label elements

Labelling

- Signal word warning

2.2.1.2 Pictograms

GHS07	
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Hazard statements	
H302	harmful if swallowed
H319	causes serious eye irritation
H412	harmful to aquatic life with long lasting effects

Precautionary statements	
P270	do not eat, drink or smoke when using this product
P273	avoid release to the environment
P280	wear protective gloves/protective clothing/eye protection/face protection/hearing protection
P301+P312	IF SWALLOWED: 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
P330	rinse mouth
P337+P313	if eye irritation persists: Get medical advice/attention
P501	dispose of contents/container in accordance with local/regional/national/international regulations

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Acetophenone-d3

Identifiers

CAS No 17537-31-4

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	500 mg/kg	oral

Molecular formula C8H5D3O

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Molar mass

123 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. Provide fresh air.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water spray, Alcohol resistant foam, BC-powder, Carbon dioxide (CO₂)

Unsuitable extinguishing media

Water jet

5.2 Special hazards arising from the substance or mixture

Hazardous combustion products

Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Co-ordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Remove persons to safety.

For emergency responders

Wear breathing apparatus if exposed to vapours/dust/spray/gases.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains

Advice on how to clean up a spill

Wipe up with absorbent material (e.g. cloth, fleece). Collect spillage: sawdust, kieselgur (diatomite), sand, universal binder

Appropriate containment techniques

Use of adsorbent materials.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations

Store in a dry place.

- Measures to prevent fire as well as aerosol and dust generation

Use local and general ventilation. Use only in well-ventilated areas.

Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

7.3 Specific end use(s)

See section 16 for a general overview.

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limit values (Workplace Exposure Limits)
this information is not available

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	22 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	6.3 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

Environmental values

Relevant PNECs and other threshold levels				
Endpoint	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0.086 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.009 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	34.6 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	1.13 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.113 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.175 mg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Appropriate engineering controls

General ventilation.

Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Skin protection

- Hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. In the case of wanting to use the gloves again, clean them before taking off and air them well. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

- Type of material

Nitrile

IIR: isobutene-isoprene (butyl) rubber

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- Breakthrough times of the glove material

>30 minutes (permeation: level 2)

- Other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended. Wash hands thoroughly after handling.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Environmental exposure controls

Use appropriate container to avoid environmental contamination. Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	not determined
Odour	characteristic
Melting point/freezing point	20 °C
Boiling point or initial boiling point and boiling range	202 °C
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	1.4 vol% - 5.2 vol%
Flash point	76 °C (c.c.) closed cup
Auto-ignition temperature	535 °C at 1,013 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	1.59 mm ² /s at 25 °C

Solubility(ies)

Water solubility	6,300 mg/l at 25 °C
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Partition coefficient

Partition coefficient n-octanol/water (log value)	1.63 (ECHA)
Soil organic carbon/water (log KOC)	0.973 (ECHA)

Vapour pressure	45 Pa at 25 °C
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Density and/or relative density

Density	1.06 g/cm ³ at 25 °C
Relative vapour density	information on this property is not available

Particle characteristics	not relevant (liquid)
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9.2 Other information

Information with regard to physical hazard classes	hazard classes acc. to GHS (physical hazards): not relevant
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Other safety characteristics

Surface tension	39 mN/m (25 °C) (ECHA)
Refractive index	1.53 (20 °C) ((lit.))

SECTION 10: Stability and reactivity

10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials".

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

Oxidisers

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10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed.

GHS of the United Nations, annex 4: May be harmful in contact with skin.

- Acute toxicity estimate (ATE)

Oral 500 mg/kg

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

11.2 Information on other hazards

There is no additional information.

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SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

12.2 Persistence and degradability

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	64.7 %	14 d
DOC removal	<30 %	28 d

12.3 Bioaccumulative potential

Data are not available.

n-octanol/water (log KOW)	1.63 (ECHA)
BCF	0.475 (ECHA)

12.4 Mobility in soil

Henry's law constant	0.766 Pa m ³ /mol at 20 °C
The Organic Carbon normalised adsorption coefficient	0.973 (ECHA)

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

Completely emptied packages can be recycled. Handle contaminated packages in the same way as the substance itself.

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Remarks

Please consider the relevant national or regional provisions. Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities.

SECTION 14: Transport information

14.1 UN number or ID number

ICAO-TI UN 3334

14.2 UN proper shipping name

ICAO-TI Aviation regulated liquid, n.o.s. (Acetophenone- β,β,β)

14.3 Transport hazard class(es)

ICAO-TI none

14.4 Packing group

ICAO-TI III

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

International Maritime Dangerous Goods Code (IMDG) - Additional information

Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Danger label(s) 9



Special provisions (SP) A27

Excepted quantities (EQ) E1

Limited quantities (LQ) 30 kg

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SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on persistent organic pollutants (POP)

Not listed.

National regulations (GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
Acetophenone-d3	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3

National inventories

Country	Inventory	Status
EU	REACH Reg.	substance is listed
US	TSCA	substance is listed

Legend

REACH Reg. REACH registered substances
TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
8.1	Control parameters: This information is not available.	Control parameters: Occupational exposure limit values (Workplace Exposure Limits) this information is not available	yes
11.1	Acute toxicity: Harmful if swallowed.GHS of the United Nations, annex 4:	Acute toxicity: Harmful if swallowed.GHS of the United Nations, annex 4: May be harmful in contact with skin.	yes

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H412	Harmful to aquatic life with long lasting effects.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.