

Chemical Safety Data Sheet MSDS / SDS

2-Phenylacetoacetonitrile

Revision Date:2026-05-31 Revision Number:1

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

Product name : 2-Phenylacetoacetonitrile
CBnumber : CB7410301
CAS : 4468-48-8
EINECS Number : 224-737-4
Synonyms : alpha-phenylacetoacetonitrile,2-Phenylacetoacetonitrile

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

Warning

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P312 Call a POISON CENTER or doctor/physician if you feel unwell.

Hazard statements

H315 Causes skin irritation
H319 Causes serious eye irritation
H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2-Phenylacetoacetonitrile
Synonyms	: alpha-phenylacetoacetonitrile, 2-Phenylacetoacetonitrile
CAS	: 4468-48-8
EC number	: 224-737-4
MF	: C ₁₀ H ₉ NO
MW	: 159.19

SECTION 4: First aid measures

Description of first aid measures

General information

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

In case of unconsciousness place patient stably in side position for transportation.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

After eye contact

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

After swallowing

Immediately call a doctor.

Most important symptoms and effects, both acute and delayed

No further relevant information available.

Indication of any immediate medical attention and special treatment needed

No further relevant information available.

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing agents

Use fire fighting measures that suit the environment.

A solid water stream may be inefficient.

Special hazards arising from the substance or mixture

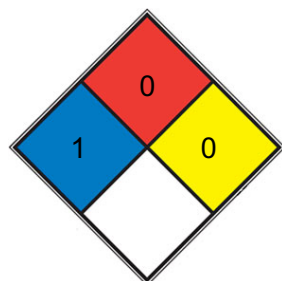
No further relevant information available.

Advice for firefighters

Protective equipment

Mouth respiratory protective device.

NFPA 704



HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete,

FIRE 0 stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N2](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Not required.

Environmental precautions

Do not allow to enter sewers/ surface or ground water.

Methods and material for containment and cleaning up

Ensure adequate ventilation.

Protective Action Criteria for Chemicals

PAC-1

Substance is not listed.

PAC-2

Substance is not listed.

PAC-3

Substance is not listed.

Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

Precautions for safe handling

Thorough dedusting.

Ensure good ventilation/exhaustion at the workplace.

Information about protection against explosions and fires

No special measures required.

Conditions for safe storage, including any incompatibilities

Storage

Store in accordance with information listed on the product insert.

Requirements to be met by storerooms and receptacles

No special requirements.

Information about storage in one common storage facility

Not required.

Further information about storage conditions

Keep receptacle tightly sealed.

Specific end use(s)

No further relevant information available.

SECTION 8: Exposure controls/personal protection

Control parameters

Components with limit values that require monitoring at the workplace

Not required.

Additional information

The lists that were valid during the creation were used as basis.

Exposure controls

Appropriate engineering controls

No further data; see section 7.

Personal protective equipment

General protective and hygienic measures

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

Breathing equipment

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

Protection of hands

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection

Tightly sealed goggles

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical State

Solid

Color

Crystals from EtOH (aq) or EtOAc/pet ether

Odor

Characteristic

Structural Formula

C₁₀H₉NO

Molecular Weight

159.2 g/mol

Storage Buffer**Odor Threshold**

Not determined.

Formulation**Melting point/Melting range**

Undetermined.

Boiling point/Boiling range

284.68°C (rough estimate)

Flammability

Product is not flammable.

Explosion limits

Lower: Not determined.

Upper: Not determined.

Flash point

Not applicable.

Decomposition temperature

Not determined.

pH

Not applicable.

Viscosity**Kinematic**

Not applicable.

SOLUBILITY

DMF: 30 mg/ml; DMF:PBS (pH 7.2); (1:7): 0.12 mg/ ml; DMSO: 25 mg/ml; Ethanol: 15 mg/ml

Dynamic

Not applicable.

Solubility in / Miscibility with

DMF: 30 mg/ml; DMF:PBS (pH 7.2); (1:7): 0.12 mg/ml; DMSO: 25 mg/ml; Ethanol: 15 mg/ml

Water

Not determined.

Partition coefficient (n-octanol/water)

Not determined.

Vapor Pressure

Not applicable.

Density

1.1202 (rough estimate)

Relative Density

1.1202 (rough estimate)

Vapor Density

Not applicable.

Particle characteristics

Not determined.

Other information

Appearance

Form

Solid

Important information on protection of health and environment, and on safety.

Ignition temperature

Not determined.

Danger of explosion

Product does not present an explosion hazard.

Change in condition

Evaporation Rate

Not applicable.

SECTION 10: Stability and reactivity

Reactivity

No further relevant information available.

Chemical stability

Thermal decomposition / conditions to be avoided

No decomposition if used according to specifications.

Possibility of hazardous reactions

No dangerous reactions known.

Conditions to avoid

No further relevant information available.

Incompatible materials

strong acids, strong bases, strong oxidizing agents

Hazardous decomposition products

carbon dioxide, carbon monoxide, nitrogen oxides

SECTION 11: Toxicological information

RTECS Number

AL7708000

Information on toxicological effects

Acute toxicity

LD/LC50 values that are relevant for classification:

Route	Endpoint	Value
Intraperitoneal	LD50	200 mg/kg (mouse)

Primary irritant effect

on the skin

Irritant to skin and mucous membranes.

on the eye

Irritating effect.

Sensitization

No sensitizing effects known.

Additional toxicological information

Interactive effects

No interactive effects between components are known.

Carcinogenic categories

IARC (International Agency for Research on Cancer)

Substance is not listed.

NTP (National Toxicology Program)

Substance is not listed.

OSHA-Ca (Occupational Safety & Health Administration)

Substance is not listed.

Alternative sources for toxicological information

No non-standard sources for toxicological information where used.

SECTION 12: Ecological information

Toxicity

Aquatic toxicity

No further relevant information available.

Persistence and degradability

No further relevant information available.

Bioaccumulative potential

No further relevant information available.

Mobility in soil

No further relevant information available.

Results of PBT and vPvB assessment

PBT

Not applicable.

vPvB

Not applicable.

Other adverse effects													
Additional ecological information:													
General notes:													
Water hazard class 1 (Self-assessment):	slightly hazardous for water												
Do not allow undiluted product or large quantities of it to reach	groundwater, watercourse or sewage												

system.

PBT:

Not applicable.

vPvB:

Not applicable.

SECTION 13: Disposal considerations

Waste treatment methods

Recommendation

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

Uncleaned packagings

Recommendation

Disposal must be made according to official regulations.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA not regulated

UN proper shipping name

DOT, IMDG, IATA not regulated

Transport hazard class(es)

DOT, ADN, IMDG, IATA

Class not regulated

Packing group

DOT, IMDG, IATA not regulated

Environmental hazards

Not applicable.

Special precautions for user

Not applicable.

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

MARPOL73/78 and the IBC Code Not applicable.

UN "Model Regulation"

not regulated

SECTION 15: Regulatory information

Chemicals known to cause developmental toxicity

Substance is not listed.

Safety, health and environmental regulations/legislation specific for the substance or mixture									
No further relevant information available.									
Sara									
Section 355 (extremely hazardous substances):	Substance is not listed.								
Section 313 (Specific toxic chemical listings):	Substance is not listed.								
TSCA (Toxic Substances Control Act):	INACTIVE								
Hazardous Air Pollutants:	Substance is not listed.								
Chemicals known to cause cancer:	Substance is not listed.								
Chemicals known to cause reproductive toxicity for females:	Substance is not listed.								
Chemicals known to cause reproductive toxicity for males:	Substance is not listed.								
						(	Contd. on page 8)		
									US

Sara

Section 355 (extremely hazardous substances):	Substance is not listed.
Section 313 (Specific toxic chemical listings):	Substance is not listed.
TSCA (Toxic Substances Control Act):	INACTIVE
Hazardous Air Pollutants:	Substance is not listed.
Chemicals known to cause cancer:	Substance is not listed.
Chemicals known to cause reproductive toxicity for females:	Substance is not listed.
Chemicals known to cause reproductive toxicity for males:	Substance is not listed.
Chemicals known to cause developmental toxicity:	Substance is not listed.

Carcinogenic categories

EPA (Environmental Protection Agency):	Substance is not listed.
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TLV (Threshold Limit Value)

Substance is not listed.

NIOSH-Ca (National Institute for Occupational Safety and Health)

Substance is not listed.

Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Acute toxicity - oral 4: Acute toxicity – Category 4

Skin irritation 2: Skin corrosion/irritation – Category 2

Eye irritation 2A: Serious eye damage/eye irritation – Category 2A

Specific target organ toxicity (single exposure) 3: Specific target organ toxicity (single exposure) – Category 3

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.