

• SAFETY DATA SHEET

Version 6.6
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 4-Phenyl-3-buten-2-one
Product Number : 147885
Brand : Aldrich
CAS-No. : 122-57-6

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

Identified uses : Laboratory chemicals, Synthesis of substances
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Skin irritation : Category 2

Skin sensitisation : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H315 Causes skin irritation.
H317 May cause an allergic skin reaction.

Precautionary statements : **Prevention:**
P261 Avoid breathing dust.
P264 Wash skin thoroughly after handling.
P272 Contaminated work clothing must not be allowed out of the workplace.
P280 Wear protective gloves.

Response:

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 122-57-6

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
4-phenyl-3-buten-2-one	122-57-6*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice	: Show this 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. Consult a physician.
In case of eye contact	: After eye contact: rinse out with plenty of water. Remove contact lenses.
If swallowed	: After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.

Vapours 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.

- Hazardous combustion products : Carbon oxides
- Specific extinguishing methods : No data available
- Further information : Prevent fire extinguishing water from contaminating surface water or the ground water system.
- Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

- Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Avoid inhalation of dusts.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.
- Environmental precautions : Do not let product enter drains.
- 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Further information on storage conditions : Tightly closed.
Dry.
- Storage class : 11, Combustible Solids
- Recommended storage : Recommended storage temperature see product label.

temperature

Further information on storage stability : Light sensitive.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts 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.

Recommended Filter type: : Filter type 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.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

Remarks : 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).

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses
- Skin and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : Solidified mass or fragments
- Color : light yellow
- Odor : No data available
- Odor Threshold : No data available
pH : No data available
- Melting point/ range : 102 - 108 °F / 39 - 42 °C
Method: lit.
- Boiling point/boiling range : 500 - 504 °F / 260 - 262 °C
Method: lit.
- Flash point : 253 °F / 123 °C
Method: closed cup
- Evaporation rate : No data available
- Flammability (solid, gas) : No data available
- Flammability (liquids) : No data available
- Burning rate : No data available
- Self-ignition : 698 °F / 370 °C
- Upper explosion limit /
Upper flammability limit : No data available
- Lower explosion limit /
Lower flammability limit : No data available

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Vapor pressure	: 0.01 hPa (77 °F / 25 °C)
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.003 g/cm ³ (113 °F / 45 °C)
Solubility(ies)	
Water solubility	: 1.3 g/l soluble (68 °F / 20 °C)
Partition coefficient: n-octanol/water	: log Pow: 2.1
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 146.19 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

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. The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : Violent reactions possible with:
Strong oxidizing agents

Conditions to avoid : Strong heating.

Incompatible materials : No data available

Hazardous decomposition products : In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 2,031 mg/kg
Remarks: Behavioral: Muscle weakness.
Vascular: Regional or general arteriolar or venous dilation.
Skin and Appendages: Other: Hair.
(RTECS)
Inhalation: Irritating to respiratory system.
LD50 Dermal - Rabbit - > 3,000 mg/kg
Remarks: (ECHA)

Skin corrosion/irritation

Skin - Guinea pig
Result: Irritating to skin. - 48 h
Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation - 24 h
(OECD Test Guideline 405)

Respiratory or skin sensitization

Patch test: - In vitro study
Result: positive
Remarks: (External MSDS)

Germ cell mutagenicity

Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: Metabolic activation
Result: negative
Remarks: (ECHA)
Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster lung cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: positive

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Test Type: comet assay
Species: Rat

Application Route: Gavage
Method: OECD Test Guideline 489
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 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

RTECS: EN0330000

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

Ecotoxicity

Components:

4-phenyl-3-buten-2-one:

Toxicity to fish : LC50 (*Oryzias latipes*): 5.7 mg/l
End point: mortality
Exposure time: 96 h
Test Type: semi-static test
Analytical monitoring: yes
Method: US-EPA
GLP: yes

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- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 15 mg/l
 End point: Immobilization
 Exposure time: 48 h
 Test Type: static test
 Analytical monitoring: yes
 Method: US-EPA
 GLP: yes
- Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata): 0.553 mg/l
 Exposure time: 72 h
 Test Type: static test
 Analytical monitoring: yes
 Method: US-EPA
 GLP: yes
- Toxicity to fish (Chronic toxicity) : NOEC (Danio rerio (zebra fish)): 0.036 mg/l
 Exposure time: 36 d
 Test Type: flow-through test
 Analytical monitoring: yes
 Method: OECD Test Guideline 210
 GLP: yes
- Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : EC50 (Daphnia magna (Water flea)): > 2.28 mg/l
 End point: Immobilization
 Exposure time: 21 d
 Test Type: semi-static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 211
 GLP: yes
- Toxicity to microorganisms : EC50 (activated sludge): 383 mg/l
 Exposure time: 3 h
 Test Type: static test
 Method: ISO 8192
 GLP: yes
 Remarks: (ECHA)

Persistence and degradability

Components:

4-phenyl-3-buten-2-one:

- Biodegradability : aerobic
 Inoculum: activated sludge
 Concentration: 100 mg/l
 Result: Readily biodegradable.
 Biodegradation: 81 %
 Exposure time: 28 d
 Method: OECD Test Guideline 301F
 GLP: yes

Bioaccumulative potential

Components:

4-phenyl-3-buten-2-one:

Partition coefficient: n- : log Pow: 2.1
octanol/water

Mobility in soil

No data available

Other adverse effects

Components:

4-phenyl-3-buten-2-one:

Additional ecological : Discharge into the environment must be avoided.
information

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards : Acute Health Hazard

SARA 313 : 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.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response;

EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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.

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