

• SAFETY DATA SHEET

Version 6.5
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 4'-(4-Bromophenyl)acetophenone

Product Number : 640468

Brand : Aldrich

CAS-No. : 5731-01-1

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

Eye irritation : Category 2A

Short-term (acute) aquatic hazard : Category 2

Long-term (chronic) aquatic hazard : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Warning

Hazard statements : H319 Causes serious eye irritation.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**

P264 Wash skin thoroughly after handling.

P273 Avoid release to the environment.

P280 Wear eye protection/ face protection.

Response:

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.

P391 Collect spillage.

Disposal:

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 5731-01-1

Components

| Chemical name | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|---|-------------------|-----------------------|--------------|
| 1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one | 5731-01-1* | >= 90 - <= 100 | - |

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.

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.

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 (CO₂)
Dry powder

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

Specific hazards during fire fighting : Combustible.

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

Hazardous combustion : Carbon oxides

products

Hydrogen bromide gas

| | |
|--|--|
| Specific extinguishing methods | : No data available |
| Further information | : Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system. |
| Special protective equipment for fire-fighters | : In the event of fire, wear self-contained breathing apparatus. |

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 temperature | : Recommended storage temperature see product label. |

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 : Handle with impervious gloves.
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 | : Change contaminated clothing. Wash hands after working with substance. |

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

| | |
|---|---|
| Appearance | : solid |
| Color | : No data available |
| Odor | : No data available |
| Odor Threshold | : No data available |
| pH | : No data available |
| Melting point/ range | : 264 - 271 °F / 129 - 133 °C Method: lit. |
| Boiling point/boiling range | : No data available |
| Flash point | : No data available |
| Evaporation rate | : No data available |
| Flammability (solid, gas) | : No data available |
| Flammability (liquids) | : No data available |
| Burning rate | : No data available |
| Upper explosion limit / Upper flammability limit | : No data available |
| Lower explosion limit / Lower flammability limit | : No data available |
| Vapor pressure | : No data available |
| Relative vapour density | : No data available |
| Relative density | : No data available |
| Density | : No data available |

| | |
|--|---------------------|
| Water solubility | : No data available |
| Partition coefficient: n-octanol/water | : log Pow: 4.397 |
| 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 | : No data available |
| Molecular weight | : 275.14 g/mol |
| Particle characteristics | |
| Particle size | : No data available |

SECTION 10. STABILITY AND REACTIVITY

| | |
|------------------------------------|---|
| Reactivity | : 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 | : No data available |
| Conditions to avoid | : no information available |
| Incompatible materials | : Strong oxidizing agents |
| Hazardous decomposition products | : In the event of fire: see section 5 |

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

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LD50 Oral - 2,500 mg/kg
Inhalation: No data available
Dermal: No data available
No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

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

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

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one:

Toxicity to fish : LC50 : 2.0 mg/l
Exposure time: 96.0 h

Remarks: No data available

Persistence and degradability

Components:

1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one:

Biodegradability : Remarks: No data available

Bioaccumulative potential

Components:

1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one:

Bioaccumulation : Remarks: No data available

Partition coefficient: n-octanol/water : log Pow: 4.397

Mobility in soil

Components:

1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one:

Stability in soil : Remarks: No data available

Other adverse effects

No data available

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

| | |
|--------------------------------------|---|
| UN/ID No. | : UN 3077 |
| Proper shipping name | : Environmentally hazardous substance, solid, n.o.s. (1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one) |
| Class | : 9 |
| Packing group | : III |
| Labels | : Class 9 - Miscellaneous dangerous substances and articles |
| Packing instruction (cargo aircraft) | : 956 |

Packing instruction : 956
(passenger aircraft)

IMDG-Code

UN number : UN 3077
Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,
N.O.S.
(1-(4'-Bromo[1,1'-biphenyl]-4-yl)ethan-1-one)
Class : 9
Packing group : III
Labels : 9
EmS Code : F-A, S-F
Marine pollutant : yes

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 : EHS-Mark required (ADR 2.2.9.1.10, IMDG code
2.10.3) for single packagings and combination
packagings containing inner packagings with
Dangerous Goods > 5L for liquids or > 5kg for solids.
Packages smaller than or equal to 5 kg / L , not
dangerous goods of Class 9

The transport classification(s) provided herein are for informational purposes only, and solely
based upon the properties of the unpackaged material as it is described within this Safety
Data Sheet. Transportation classifications may vary by mode of transportation, package
sizes, and variations in regional or country 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 : Product contains substance(s) not listed on 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

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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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