

## SAFETY DATA SHEET

Version 5.6  
Revision Date 08/24/2016  
Print Date 10/20/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 4'-Isobutylacetophenone

Product Number : PHR1146  
Brand : Sigma-Aldrich

CAS-No. : 38861-78-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

## 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226  
Skin sensitisation (Category 1), H317  
Acute aquatic toxicity (Category 2), H401  
Chronic aquatic toxicity (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Warning

Hazard statement(s)

H226 : Flammable liquid and vapour.  
H317 : May cause an allergic skin reaction.  
H411 : Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 : Keep away from heat/sparks/open flames/hot surfaces. No smoking.  
P233 : Keep container tightly closed.  
P240 : Ground/bond container and receiving equipment.  
P241 : Use explosion-proof electrical/ ventilating/ lighting/ equipment.  
P242 : Use only non-sparking tools.  
P243 : Take precautionary measures against static discharge.

P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms : 4'-Isobutylacetophenone  
1-(4-Isobutylphenyl)ethanone  
1-Acetyl-4-isobutylbenzene

Formula : C<sub>12</sub>H<sub>16</sub>O  
Molecular weight : 176.25 g/mol  
CAS-No. : 38861-78-8  
EC-No. : 254-159-8

#### Hazardous components

Component	Classification	Concentration
<b>1-[4-(2-methylpropyl)phenyl]ethan-1-one</b>		
	Flam. Liq. 3; Skin Sens. 1; Aquatic Acute 2; Aquatic Chronic 2; H226, H317, H411	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature 2 - 8 °C

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### **Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

Hazardous components without workplace control parameters

### 8.2 Exposure controls

#### **Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

## Personal protective equipment

### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |                                   |
|---|-----------------------------------|
| a) Appearance                                   | Form: liquid                      |
| b) Odour  | No data available                 |
| c) Odour Threshold                              | No data available                 |
| d) pH   | No data available                 |
| e) Melting point/freezing point                 | No data available                 |
| f) Initial boiling point and boiling range      | 107 °C (225 °F) at 3 hPa (2 mmHg) |
| g) Flash point                                  | 54.4 °C (129.9 °F)                |
| h) Evaporation rate                             | No data available                 |
| i) Flammability (solid, gas)                    | No data available                 |
| j) Upper/lower flammability or explosive limits | No data available                 |
| k) Vapour pressure                              | No data available                 |
| l) Vapour density                               | No data available                 |
| m) Relative density                             | 0.96 g/cm <sup>3</sup>            |
| n) Water solubility                             | partly miscible                   |
| o) Partition coefficient: n-octanol/water       | log Pow: 3.59 at 21 °C (70 °F)    |
| p) Auto-ignition temperature                    | No data available                 |
| q) Decomposition temperature                    | No data available                 |
| r) Viscosity                                    | No data available                 |
| s) Explosive properties                         | No data available                 |

t) Oxidizing properties      No data available

## 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Reducing agents, Strong oxidizing agents, Strong bases

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - 5,000 mg/kg

LD50 Oral - Rat - > 2,000 mg/kg  
(OECD Test Guideline 401)

LD50 Oral - Mouse - male - > 1,600 mg/kg

Remarks: Gastrointestinal disturbance

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Mild eye irritation

#### Respiratory or skin sensitisation

Buehler Test - Guinea pig

May cause sensitisation by skin contact.  
(OECD Test Guideline 406)

#### Germ cell mutagenicity

Not mutagenic in Ames Test

#### 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 identified as a carcinogen or potential carcinogen by OSHA.

## **Reproductive toxicity**

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

### **Additional Information**

RTECS: Not available

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

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## **12. ECOLOGICAL INFORMATION**

### **12.1 Toxicity**

Toxicity to fish                      static test LC50 - Cyprinodon variegatus (sheepshead minnow) - 10 - 30 mg/l - 96 h

static test LC50 - Lepomis macrochirus (Bluegill) - 12.4 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates                      static test EC50 - Daphnia (water flea) - 7.7 mg/l - 48 h

static test EC50 - other microorganisms - 0.3 - 3.0 mg/l - 96 h

Toxicity to algae                      static test IC50 - Algae - 4.0 mg/l - 96 h

static test IC50 - Skeletonema costatum (marine diatom) - 7.0 mg/l - 96 h

Toxicity to bacteria                      LC50 - Photobacterium phosphoreum - 0.63 mg/l - 0.4 h

### **12.2 Persistence and degradability**

Biodegradability                      aerobic - Exposure time 28 d  
Result: 10 - 60 % - Not readily biodegradable.  
(OECD Test Guideline 301)

### **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 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Toxic to aquatic life with long lasting effects.

No data available

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## **13. DISPOSAL CONSIDERATIONS**

### **13.1 Waste treatment methods**

#### **Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

#### **Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 1224      Class: 3      Packing group: III  
Proper shipping name: Ketones, liquid, n.o.s. (1-[4-(2-methylpropyl)phenyl]ethan-1-one)  
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

UN number: 1224      Class: 3      Packing group: III      EMS-No: F-E, S-D  
Proper shipping name: KETONES, LIQUID, N.O.S. (1-[4-(2-methylpropyl)phenyl]ethan-1-one)

### IATA

UN number: 1224      Class: 3      Packing group: III  
Proper shipping name: Ketones, liquid, n.o.s. (1-[4-(2-methylpropyl)phenyl]ethan-1-one)

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## 15. REGULATORY INFORMATION

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

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.

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1-[4-(2-methylpropyl)phenyl]ethan-1-one	38861-78-8	

### New Jersey Right To Know Components

	CAS-No.	Revision Date
1-[4-(2-methylpropyl)phenyl]ethan-1-one	38861-78-8	

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H317	May cause an allergic skin reaction.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
Skin Sens.	Skin sensitisation

### HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	2
Physical Hazard	0

**NFPA Rating**

Health hazard: 2

Fire Hazard: 2

Reactivity Hazard: 0

**Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

**Preparation Information**

Sigma-Aldrich Corporation

Product Safety – Americas Region

1-800-521-8956

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