ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

4'-(2-Methylpropyl)acetophenone

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

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

Product identifier

Product name	: 4'-(2-Methylpropyl)acetophenone
CBnumber	: CB3210390
CAS	: 38861-78-8
EINECS Number	: 254-159-8
Synonyms	: 4-isobutylacetophenone,1-(4-isobutylphenyl)ethan-1-one

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

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P273 Avoid release to the environment.

P272 Contaminated work clothing should not be allowed out of the workplace.

P264 Wash skin thouroughly after handling.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H411 Toxic to aquatic life with long lasting effects

H317 May cause an allergic skin reaction

H315 Causes skin irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4'-(2-Methylpropyl)acetophenone
Synonyms	: 4-isobutylacetophenone,1-(4-isobutylphenyl)ethan-1-one
CAS	: 38861-78-8
EC number	: 254-159-8
MF	: C12H16O
MW	: 176.25

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) 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

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. 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

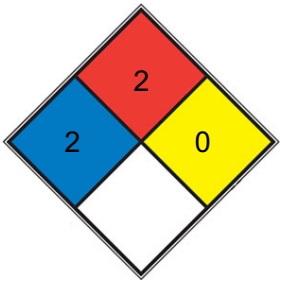
Specific extinguishing methods

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.

NFPA 704



■	HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. diethyl ether, ammonium phosphate, iodine)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■	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

Advice for non-emergency personnel: Do not breathe vapours, aerosols. 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7: Handling and storage

Handling

Avoidance of contact

Reducing agents Strong oxidizing agents Strong bases

Storage

Further information on storage conditions

Tightly closed.

Storage class

10, Combustible liquids

Recommended storage temperature

-70°C Degree Freezer

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 vapours/aerosols 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 ABEK

The entrepeneur 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.

Eye/face 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

Hand protection

Remarks

required

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

clear, colourless

Odor

No data available

Odor Threshold

No data available

pH

No data available

pH

6.2

Method: OECD Test Guideline 105

GLP: yes

pH

6

Method: OECD Test Guideline 117

GLP: yes Bioaccumulation is not expected.

Melting point/ range

-13 °C (1,013 hPa)

Method: OECD Test Guideline 102

GLP: yes

Boiling point/boiling range

266.9 °C (1,013 hPa)

Method: OECD Test Guideline 103

GLP: yes

Flash point

141.5 °C (1,007 hPa)

Method: Regulation (EC) No. 440/2008, Annex, A.9, closed cup

GLP: yes

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Self-ignition

461 °C 1,020 hPa

GLP: yes

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

< 0.1 hPa (20 °C)

Method: OECD Test Guideline 104

GLP: yes

Relative vapor density

No data available

Relative density

0,952 g/cm^3

Density

0.95 g/cm3 (20 °C)

Method: OECD Test Guideline 109

GLP: yes

Water solubility

75 g/l (20 °C)

Partition coefficient: n-octanol/water

log Pow: 3.4 (23 °C)

Autoignition temperature

> 570 °C

Decomposition temperature Viscosity: No data available

Viscosity, dynamic

5.35 mPa.s (20 °C)

Method: OECD Test Guideline 114

GLP: yes

Viscosity, kinematic

5.31 mm2/s (20 °C)

Method: OECD Test Guideline 114

GLP: yes

Flow time

No data available

Explosive properties

Not classified as explosive.

Oxidizing properties

none

Molecular weight

176.25 g/mol

Particle characteristics Particle size

No data available

Solubility

soluble in Dichloromethane; Diethyl Ether; Ethyl Acetate; THF

Physical state

liquid

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.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

No data available

Conditions to avoid

Strong heating.

Incompatible materials

Reducing agents Strong oxidizing agents Strong bases

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 - male and female - > 2,000 mg/kg (OECD Test Guideline 401)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Skin - in vitro assay

Result: Irritating to skin. - 0.5 h (OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - In vitro study

Result: No eye irritation - 0.5 h (OECD Test Guideline 437)

Respiratory or skin sensitization

Maximisation Test - Guinea pig

The product is a skin sensitiser, sub-category 1B.

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

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-(2-methylpropyl)phenyl]ethan-1-one:

Toxicity to fish

LC50 (Cyprinodon variegatus (sheepshead minnow)): 10 - 30 mg/l Exposure time: 96 h Test Type: static test

Toxicity to daphnia and other aquatic invertebrates

EC50 (Daphnia magna (Water flea)): 4.92 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes EC50 (other microorganisms): 0.3 - 3.0 mg/l Exposure time: 96 h Test Type: static test EC50 (Daphnia (water flea)): 7.7 mg/l Exposure time: 48 h Test Type: static test

Toxicity to algae/aquatic plants

NOEC (Pseudokirchneriella subcapitata): 1.69 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes EC50 (Pseudokirchneriella subcapitata): 5.11 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes

Toxicity to microorganisms

EC50 (activated sludge): 280 mg/l Exposure time: 3 h Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

1-[4-(2-methylpropyl)phenyl]ethan-1-one:

Biodegradability

aerobic Inoculum: activated sludge, non-adapted Concentration: 20 mg/l Result: Not readily biodegradable. Biodegradation: 50 - 60 % Exposure time: 28 d Method: OECD Test Guideline 301B GLP: yes

Bioaccumulative potential

Components:

1-[4-(2-methylpropyl)phenyl]ethan-1-one:

Partition coefficient: noctanol/water

log Pow: 3.4 (23 °C) pH: 6 Method: OECD Test Guideline 117 GLP: yes Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 3082

Proper shipping name : Environmentally hazardous substance, liquid, n.o.s.

(1-[4-(2-methylpropyl)phenyl]ethan-1-one)

Class : 9

Packing group : III

Labels : Class 9 - Miscellaneous dangerous substances and articles

Packing instruction (cargo aircraft) : 964

Packing instruction (passenger aircraft) : 964

IMDG-Code

UN number : UN 3082

Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

(1-[4-(2-methylpropyl)phenyl]ethan-1-one)

Class : 9

Packing group : III

Labels : 9

EmS Code : F-A, S-F

Marine pollutant : yes

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National Regulations

JT/T 617

UN number : UN 3082

Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

(1-[4-(2-methylpropyl)phenyl]ethan-1-one)

Class : 9

Packing group : III

Labels : 9

Environmentally hazardous : 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

Catalogue of Hazardous Chemicals : This product is not listed in the catalogue of hazardous chemicals, but it meets the definition of hazardous chemicals and its principles of determination.
Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Not listed

Hazardous Chemicals for Priority Management

Not listed under SAWS

Catalogue of Specially Controlled Hazardous

Not listed Chemicals

List of Explosive Precursors

Not listed

Regulations on Labour Protection in Workplaces where Toxic Substances are Used

Catalogue of Highly Toxic Chemicals

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A222211051 B1A222223646

Regulation on the Administration of Precursor Chemicals

Catalogue and Classification of Precursor Chemicals

Not listed

Regulations on the Administration of Controlled Chemicals

List of Controlled Chemicals

Not listed

Regulations of Ozone Depleting Substances Management

List of Controlled Ozone Depleting Substances

Not listed

List of Controlled Ozone Depleting Substances Import and Export

Not listed

Environmental Protection Law

List of Priority Controlled Chemicals

Not listed

List of Key Controlled New Pollutants

Not listed

SECTION 16: Other information

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency forTransport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN -Standard of the German Institute for Standardisation

DSL - Domestic SubstancesList (Canada)

ECx - Concentration associated with x% response

ELx - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and NewChemical Substances (Japan)

ErCx - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonised System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Can- cer

IATA - International Air Transport Association

IBC - International Code for theConstruction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC50 -Half maximal inhibitory concentration

ICAO - International Civil Aviation Organiza- tion

IECSC - Inventory of Existing Chemical Substances in China

IMDG - Interna- tional Maritime Dangerous Goods

IMO - International Maritime Organisation

ISHL -Industrial Safety and Health Law (Japan)

ISO - International Organisation forStandardisation

KECI - Korea Existing Chemicals Inventory

LC50 - Lethal Concen- tration 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 Pol- lution from Ships

MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods

n.o.s. - Not Otherwise Specified

Nch - Chilean Norm

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Ef- fect Level

NOELR - No Observable Effect Loading Rate

NOM - Official MexicanNorm

NTP - National Toxicology Program

NZIoC - New Zealand Inventory of Chem- icals

OECD - Organisation for Economic Co-operation and Development

OPPTS - Of- fice of Chemical Safety and Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic substance

PICCS - Philippines Inventory of Chemicals and Chemical Sub- stances

(Q)SAR - (Quantitative) Structure Activity Relationship

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning theRegistration, Evaluation, Authorisation and Restriction of Chemicals

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - TaiwanChemical Substance Inventory

TDG - Transportation of Dangerous Goods

TECI -Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (UnitedStates)

UN - United Nations

UNRTDG - United Nations Recommendations on theTransport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

WHMIS - Workplace Hazardous Materials Information System

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.