

Chemical Safety Data Sheet MSDS / SDS

4-(4-Methoxyphenyl)-2-butanoneRevision Date:2024-12-21 Revision Number:1

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

Product name : 4-(4-Methoxyphenyl)-2-butanone
CBnumber : CB7731013
CAS : 104-20-1
EINECS Number : 203-184-2
Synonyms : Anisylacetone,4-(4-Methoxyphenyl)butan-2-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 : 400-158-6606

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Signal word : No signal word

Hazard statement(s)

none

Prevention

none

Response

none

Storage

none

Disposal

none

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4-(4-Methoxyphenyl)-2-butanone
Synonyms	: Anisylacetone, 4-(4-Methoxyphenyl)butan-2-one
CAS	: 104-20-1
EC number	: 203-184-2
MF	: C11H14O2
MW	: 178.23

SECTION 4: First aid measures

Description of first aid measures

If inhaled

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

In case of skin contact

Wash off with soap and plenty of water.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

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

Special hazards arising from the substance or mixture

Carbon oxides

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704





<input type="checkbox"/> HEALTH	0	Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials
<hr/>		
<input type="checkbox"/> FIRE	1	Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. mineral oil , ammonia)
<hr/>		
<input type="checkbox"/> REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
<hr/>		
<input type="checkbox"/> SPEC.		
<input type="checkbox"/> HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid breathing vapours, mist or gas. For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Store in cool place. 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.

Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

General industrial hygiene practice.

Personal protective equipment

Eye/face protection

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Impervious 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

Respiratory protection not required. For nuisance exposures use type OV/AG (US) or type ABEK (EU EN 14387) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance light yellow liquid, clear

Odour No data available

Odour Threshold No data available

pH No data available

Melting point/freezing point Melting point/range: 8 °C - lit.

Initial boiling point and boiling range 152 - 153 °C at 20 hPa - lit.

Flash point >113,00 °C - closed cup

Evaporation rate No data available

Flammability (solid, gas) No data available

Upper/lower flammability or explosive limits No data available

limits

Vapour pressure No data available

Vapour density No data available

Relative density	1,046 g/cm ³ at 25 °C
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents

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

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - > 5.000 mg/kg

LD50 Dermal - Rabbit - > 5.000 mg/kg

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

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.

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

Additional Information

RTECS: EL9085500

toxicity

Both the acute oral LD₅₀ value in rats and the acute dermal LD₅₀ value in rabbits exceeded 5 g/kg (Russell, 1973)

SECTION 12: Ecological information

Toxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

SECTION 14: Transport information

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

UN number

ADR/RID: 2585 IMDG: 2585 IATA: 2585

ADR/RID: 2742 IMDG: 2742 IATA: 2742

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3077 IMDG: 3077 IATA: 3077

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 3077 IMDG: 3077 IATA: 3077

ADR/RID: 2789 IMDG: 2789 IATA: 2789

ADR/RID: - IMDG: - IATA: -

ADR/RID: 2554 IMDG: 2554 IATA: 2554

UN proper shipping name

ADR/RID: METHYLALLYL CHLORIDE IMDG: METHYL ALLYL CHLORIDE IATA: Methylallyl chloride

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

ADR/RID: ACETIC ACID, GLACIAL IMDG: ACETIC ACID, GLACIAL IATA: Acetic acid, glacial

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (9,10-Dichloro- 1,2,3,4,5,6,7,8-octafluoroanthracene) IMDG:

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (9,10-Dichloro- IATA: Environmentally hazardous substance, solid, n.o.s.

1,2,3,4,5,6,7,8-octafluoroanthracene) (9,10-Dichloro-

ADR/RID: II IMDG: II IATA: II

ADR/RID: - IMDG: - IATA: -

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2-Amino-5- bromopyrimidine) IMDG: ENVIRONMENTALLY

HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2-Amino-5- IATA: Environmentally hazardous substance, solid, n.o.s. bromopyrimidine)

ADR/RID: - IMDG: - IATA: -

ADR/RID: CHLOROFORMATES, TOXIC, CORROSIVE, FLAMMABLE, N.O.S. (1-Chloroethyl chloroformate) IMDG: CHLOROFORMATES,

TOXIC, CORROSIVE, FLAMMABLE, N.O.S. (1-Chloroethyl chloroformate) IATA: Chloroformates, toxic, corrosive, flammable, n.o.s.

chloroformate)

ADR/RID: ARYLSULPHONIC ACIDS, SOLID IMDG: ARYLSULPHONIC ACIDS, SOLID IATA: Arylsulphonic acids, solid

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

(1-Chloroethyl ADR/RID: 6.1 (3, 8) IMDG: 6.1 (3, 8) IATA: 6.1 (3)(8)

ADR/RID: no IMDG Marine pollutant: no IATA: no

(2-Amino-5- ADR/RID: 9 IMDG: 9 IATA: 9

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: 9 IMDG: 9 IATA: 9

ADR/RID: - IMDG: - IATA: -

ADR/RID: 8 (3) IMDG: 8 (3) IATA: 8 (3)

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: II IMDG: II IATA: II

ADR/RID: - IMDG: - IATA: -

ADR/RID: II IMDG: II IATA: II

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

No data available

ADR/RID: III IMDG: III IATA: III

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes bromopyrimidine) Special precautions for user Further information 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.

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes 1,2,3,4,5,6,7,8-octafluoroanthracene) Special precautions for user Further information 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.

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

No data available

No data available

No data available

No data available

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

[1] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

[2] ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

[3] ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

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.