

Chemical Safety Data Sheet MSDS / SDS

1,3-DIMETHYLBUTYL ACETATE

Revision Date:2024-03-16 Revision Number:1

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

Product name : 1,3-DIMETHYLBUTYL ACETATE
CBnumber : CB8373308
CAS : 108-84-9
EINECS Number : 203-621-7
Synonyms : 4-methylpentan-2-yl acetate,methyl amyl acetate

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**Classification of the substance or mixture**

Flammable liquids, Category 3

Label elements**Pictogram(s)**

☐

Signal word : Warning

Hazard statement(s)

H226 Flammable liquid and vapour

H315 Causes skin irritation

H320 Causes eye irritation

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.

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

P264 Wash hands thoroughly after handling.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P370+P378 In case of fire: Use ... for extinction.
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P501 Dispose of contents/container to.....

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1,3-DIMETHYLBUTYL ACETATE
Synonyms	: 4-methylpentan-2-yl acetate,methyl amyl acetate
CAS	: 108-84-9
EC number	: 203-621-7
MF	: C8H16O2
MW	: 144.21

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth.

Most important symptoms and effects, both acute and delayed

Headache, dizziness, nausea, irritation to respiratory passages. Irritates eyes. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

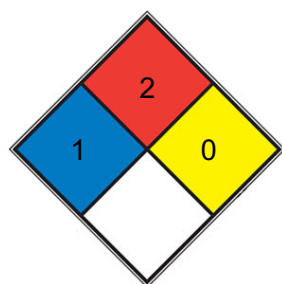
If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use foam, dry chemical, or carbon dioxide.

Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 130 [Flammable Liquids (Water-Immiscible / Noxious)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

Advice for firefighters

Use water spray, powder, alcohol-resistant foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

NFPA 704

■ HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely

■ FIRE 2 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

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

1. remove all ignition sources. 2. ventilate area of spill or leak. 3. for small quantities, absorb on paper towels. evaporate in a safe place (such as a fume hood). allow sufficient time for evaporating vapors to completely clear the hood ductwork. burn the paper in a suitable location away from combustible materials. liquid sec-hexyl acetate should not be allowed to enter a confined space, such as a sewer, because of the possibility of an explosion.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 45°C use a closed system, ventilation and explosion-proof electrical equipment. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants. Store in a cool place, away from sources of ignition.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 50 ppm as TWA

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Clear liquid
Colour	Colorless liquid with a fruity odor
Odour	Mild, pleasant, fruity odor.
Melting point/freezing point	-63.8°C
Boiling point or initial boiling point and boiling range	144°C
Flammability	Class II Combustible Liquid: Fl.P. at or above 100°F and below 140°F.
Lower and upper explosion limit/flammability limit	Flammable Limits in Air: 0.9%-5.7% (calculated)
Flash point	45°C(lit.)
Auto-ignition temperature	510° F (USCG, 1999)
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	Viscosity coefficient = 0.93 cP at 20 deg C
Solubility	Soluble in alcohol and ether (Weast, 1986).
Partition coefficient n-octanol/water	no data available
Vapour pressure	4 (NIOSH, 1997)
Density and/or relative density	0.86 g/cm ³
Relative vapour density	5.0 (AIR= 1)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with strong oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

MODERATE FIRE RISK. METHYLAMYL ACETATE is an ester. Esters react with acids to liberate heat along with alcohols and acids. Strong oxidizing acids may cause a vigorous reaction that is sufficiently exothermic to ignite the reaction products. Heat is also generated by the interaction of esters with caustic solutions. Flammable hydrogen is generated by mixing esters with alkali metals and hydrides. This compound is incompatible with the following: Nitrates; strong oxidizers, alkalis & acids (NIOSH, 2016).

Conditions to avoid

no data available

Incompatible materials

Nitrates; strong oxidizers, alkalis and acids.

Hazardous decomposition products

Toxic gases and vapors (such as carbon monoxide) may be released in a fire involving sec-hexyl acetate.

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. Exposure at high levels could cause unconsciousness.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

In aerobic screening tests using an unacclimated sewage seed, 4-methyl-2-pentyl acetate reached 20, 87, 62 and 69% of its theoretical BOD after 5, 10, 15, and 20 days, respectively in freshwater(1). In aerobic screening tests using synthetic seawater with added raw wastewater, 4-methyl-2-pentyl acetate reached 11, 22, 52, and 67% of its theoretical BOD after 5, 10, 15, and 20 days, respectively(1).

Bioaccumulative potential

An estimated BCF of 66 was calculated for 4-methyl-2-pentyl acetate(SRC), using an estimated log Kow of 2.7(1,SRC) and a recommended regression-derived equation(2). According to a classification scheme(3), this BCF suggests that bioconcentration in aquatic organisms is moderate, not high(SRC).

Mobility in soil

The Koc of 4-methyl-2-pentyl acetate is estimated as approximately 700(SRC), using an estimated log Kow of 2.7(1,SRC) and a regression-derived equation(2,SRC). According to a recommended classification scheme(3), this estimated Koc value suggests that 4-methyl-2-pentyl acetate is expected to have low mobility in soil(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible

for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1233 (For reference only, please check.)

IMDG: UN1233 (For reference only, please check.)

IATA: UN1233 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: METHYLAMYL ACETATE (For reference only, please check.)

IMDG: METHYLAMYL ACETATE (For reference only, please check.)

IATA: METHYLAMYL ACETATE (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Not Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

Listed.

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

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

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

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

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en

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

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

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

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

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

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

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