Chemical Safety Data Sheet MSDS / SDS

Methyl 3-aminocrotonate

Revision Date:2024-04-20 Revision Number:1

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

Product identifier

| Product name | : Methyl 3-aminocrotonate | | | | |
|---|--|--|--|--|--|
| CBnumber | : CB2222855 | | | | |
| CAS | : 14205-39-1 | | | | |
| EINECS Number | : 238-056-5 | | | | |
| Synonyms | : METHYL 3-AMINOCROTONATE, methyl (Z)-3-aminobut-2-enoate | | | | |
| 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

Symbol(GHS)



Signal word

Warning

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

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

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thouroughly after handling.

P264 Wash hands thoroughly after handling.

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

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Hazard statements

H335 May cause respiratory irritation

H332 Harmful if inhaled

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H315 Causes skin irritation

H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients

Substance

| Product name | : Methyl 3-aminocrotonate |
|--------------|---|
| Synonyms | : METHYL 3-AMINOCROTONATE, methyl (Z)-3-aminobut-2-enoate |
| CAS | : 14205-39-1 |
| EC number | : 238-056-5 |
| MF | : C5H9NO2 |
| MW | : 115.13 |
| | |

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

lf 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

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

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, Nitrogen oxides (NOx) Combustible.

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704

| 2 | ^ 1 ✓ | 0 |
|---------------|-------------|--|
| HEALTH | 2 | Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. <u>diethyl</u> <u>ether</u> , ammonium phosphate, iodine) |
| 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) |
| REACT | 0 | Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2) |
| SPEC. HAZ. | Ner | |

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

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.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

Reference to other sections

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

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

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.

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

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:Dermatril? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:Dermatril? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved

gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, 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 particle respirator type N100 (US) or type P3 (EN 143) 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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| Appearance | yellow solid |
|---|--|
| Odour | ammoniacal |
| Odour Threshold | No data available |
| рН | 8 - 9 at 18 g/l at 20 °C |
| Melting point/freezing point | Melting point/range: 81 - 83 °C - lit. |
| Initial boiling point and boiling range | 112 °C at 55 hPa |
| Flash point | 101 °C - closed cup |
| Evaporation rate | No data available |
| Flammability (solid, gas) | No data available |
| Upper/lower flammability or explosive | No data available |
| limits | |
| Vapour pressure | No data available |
| Vapour density | No data available |
| Relative density | No data available |
| Water solubility | 18 g/l at 20 °C |
| Partition coefficient: n-octanol/water | log Pow: -0,27 at 25 °C - Bioaccumulation is not expected. |
| 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

Solubility in other solvents

Chloroform at 20 °C

- soluble

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

No data available

Acute toxicity

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

LD50 Oral - Rat - male and female - 1.760 mg/kg Remarks: (ECHA) LC50 Inhalation - Rat - male and female - 4 h - > 0,023 mg/l Remarks: An LC50/inhalation/4h/rat could not be determined because no mortality of rats was observed at the maximum achievable concentration. (ECHA) LD50 Dermal - Rat - > 2.000 mg/kg (OECD Test Guideline 402) Skin corrosion/irritation Skin - Rabbit Result: slight irritation - 4 h (OECD Test Guideline 404) Remarks: Based on available data, the classification criteria are not met. Serious eye damage/eye irritation Eyes - Rabbit Result: Irreversible effects on the eye (OECD Test Guideline 405) Respiratory or skin sensitisation Sensitisation test (Magnusson and Kligman): - Guinea pig Result: positive (OECD Test Guideline 406) Germ cell mutagenicity

Ames test

Salmonella typhimurium Result: negative

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

Specific target organ toxicity - single exposure Specific target organ toxicity - repeated exposure Aspiration hazard

Additional Information

RTECS: EM9092500

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

Under given conditions, contact with nitrites or nitric acid can lead to the formation of nitrosamines, which have shown themselves to be carcinogenic in animal experiments. Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

Toxicity

Toxicity to fish

LC50 - Oncorhynchus mykiss (rainbow trout) - 35,4 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to bacteria

static test EC50 - activated sludge - 11.400 mg/l - 3 h (OECD Test Guideline 209)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d Result: 98 % - Readily biodegradable. (OECD Test Guideline 301B)

Bioaccumulative potential

Mobility in soil

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Harmful to aquatic life.

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Product

Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

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

Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

Packaging group

ADR/RID: - IMDG: - IATA: -

Environmental hazards

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

Special precautions for user

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

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

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

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

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

EC Inventory:Listed.

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

Chemical Book

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/ Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

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] ChemlDplus, 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:

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