

Chemical Safety Data Sheet MSDS / SDS

TRANS-2-BUTENOIC ACID

Revision Date:2024-12-21 Revision Number:1

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

Product name : TRANS-2-BUTENOIC ACID
CBnumber : CB6145402
CAS : 107-93-7
EINECS Number : 203-533-9
Synonyms : CROTONIC ACID,(E)-but-2-enoic acid

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

Danger

Precautionary statements

P501 Dispose of contents/container to.....
P406 Store in corrosive resistant/... container with a resistant inner liner.
P405 Store locked up.
P390 Absorb spillage to prevent material damage.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P234 Keep only in original container.

Hazard statements

H318 Causes serious eye damage

H314 Causes severe skin burns and eye damage

H311 Toxic in contact with skin

H302 Harmful if swallowed

H290 May be corrosive to metals

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|--|
| Product name | : TRANS-2-BUTENOIC ACID |
| Synonyms | : CROTONIC ACID,(E)-but-2-enoic acid |
| CAS | : 107-93-7 |
| EC number | : 203-533-9 |
| MF | : C ₄ H ₆ O ₂ |
| MW | : 86.09 |

SECTION 4: First aid measures

Description of first aid measures

General advice

Show this material 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.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. 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 2.2) 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

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Carbon oxides Combustible.

Vapors 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.

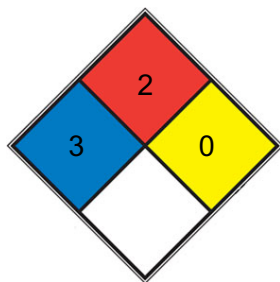
Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704



| | | | |
|-------------------------------------|--------|---|--|
| <input checked="" type="checkbox"/> | HEALTH | 3 | Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid) |
| <input checked="" type="checkbox"/> | 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) |
| <input checked="" type="checkbox"/> | REACT | 0 | Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N₂) |
| <input type="checkbox"/> | SPEC. | | |
| <input type="checkbox"/> | HAZ. | | |

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

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

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). Tightly fitting safety goggles

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved
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gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

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

Material tested:KCL 741 Dermatril? L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact Material: Nitrile rubber

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

Material tested:KCL 741 Dermatril? L

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when dusts 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 P2

The entrepreneur 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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| | |
|--|--|
| Appearance | white flakes |
| Odour | No data available |
| Odour Threshold | No data available |
| pH | 3 (10g/l, H ₂ O, 20°C) |
| Melting point/freezing point | Melting point/range: 70 - 72 °C - lit. |
| Initial boiling point and boiling range | 180 - 181 °C - lit. |
| Flash point | 88 °C - closed cup |
| Evaporation rate | No data available |
| Flammability (solid, gas) | No data available |
| Upper/lower flammability or explosive limits | Upper explosion limit: 15,1 %(V) Lower explosion limit: 2,2 %(V) |
| Vapour pressure | 0,25 hPa at 20 °C |
| Vapour density | 2.97 (vs air) |
| Relative density | 1,027 g/cm ³ at 25 °C |
| Water solubility | 94 g/l at 25 °C |

| | |
|--|---|
| Partition coefficient: n-octanol/water | log Pow: 0,71 at 25 °C - Bioaccumulation is not expected., (ECHA) |
| Autoignition temperature | >400 °C at 1.013 hPa |
| Decomposition temperature | No data available |
| Viscosity | Viscosity, kinematic: No data available Viscosity, dynamic: 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

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents peroxi compounds alkalines

strong reducing agents

Conditions to avoid

Strong heating.

Incompatible materials

No data available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 2.610 mg/kg

(OECD Test Guideline 401)

LD50 Dermal - Rat - > 2.000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage. (OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: Does not cause skin sensitization. (OECD Test Guideline 429)

Germ cell mutagenicity

gene mutation test

Chinese hamster ovary cells Result: negative

Chromosome aberration test in vitro Chinese hamster lung cells

Result: negative Ames test

S. typhimurium Result: negative

Carcinogenicity

IARC: No ingredient 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

Toxicity

LD50 orally in rats: 1.0 g/kg (Smyth, Carpenter)

SECTION 12: Ecological information

Toxicity**Toxicity to fish**

flow-through test LC50 - Pimephales promelas (fathead minnow) - 31 mg/l - 96 h
(OECD Test Guideline 203)

flow-through test NOEC - Pimephales promelas (fathead minnow) - 22 mg/l - 96 h
(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 150 mg/l - 48 h (OECD Test Guideline 202)

NOEC - Daphnia magna (Water flea) - 110 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

static test EC50 - Pseudokirchneriella subcapitata (green algae) - > 57,5 mg/l - 72 h

(OECD Test Guideline 201)

static test NOEC - Pseudokirchneriella subcapitata (green algae) - 57,5 mg/l - 72 h

(OECD Test Guideline 201)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 100 % - Readily biodegradable. (OECD Test Guideline 301F)

Bioaccumulative potential

No data available

Mobility in soil

No data available

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

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

UN number

ADR/RID: 2823 IMDG: 2823 IATA: 2823

UN proper shipping name

| | | |
|------|--|-----------|
| | ADR/RID: CROTONIC ACID, SOLID IMDG: CROTONIC ACID, SOLID | |
| | IATA: Crotonic acid, solid | |
| 14.3 | Transport hazard class(es) ADR/RID: 8 IMDG: 8 | IATA: 8 |
| 14.4 | Packaging group ADR/RID: III IMDG: III | IATA: III |
| 14.5 | Environmental hazards ADR/RID: no IMDG Marine pollutant: no | IATA: no |

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:Not Listed. website: <https://www.epa.gov/>

EC Inventory:Listed.

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/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

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

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/>

Other Information

The CAS number of unspecified crotonic acid is 3724-65-0 and cis-crotonic acid has CAS 503-64-0. The trans isomer is also called just crotonic acid, while the cis isomer is called isocrotonic acid. Commercially (unspecified) crotonic acid consists mainly (or even completely) of the trans isomer. Synonyms of unspecified crotonic acid are: alpha-crotonic acid, beta-methylacrylic acid and 3-methylacrylic acid. In general the substance will be transported as molten liquid.

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.