

Chemical Safety Data Sheet MSDS / SDS

BOC-3-iodo-D-ALANINE METHYL ESTERRevision Date:2025-07-05 Revision Number:1

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

Product name : BOC-3-iodo-D-ALANINE METHYL ESTER
CBnumber : CB4264345
CAS : 170848-34-7
Synonyms : (S)-Methyl 2-((tert-butoxycarbonyl)amino)-3-iodopropanoate,methyl (2R)-2-[(tert-butoxycarbonyl)amino]-3-iodopropanoate

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**

Signal word : no data available

Hazard statement(s)

no data available

Prevention

no data available

Response

no data available

Storage

no data available

Disposal

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: BOC-3-iodo-D-ALANINE METHYL ESTER
Synonyms	: (S)-Methyl 2-((tert-butoxycarbonyl)amino)-3-iodopropanoate, methyl (2R)-2-[(tert-butoxycarbonyl)amino]-3-iodopropanoate
CAS	: 170848-34-7
MF	: C ₉ H ₁₆ INO ₄
MW	: 329.13

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.

If 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

Flush eyes with water as a precaution.

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 (NO_x), Hydrogen iodide

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. 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

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Provide appropriate exhaust ventilation at places where dust is formed. 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. Recommended storage temperature 2 - 8 °C

Store under inert gas. Light sensitive. Moisture sensitive.

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

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

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place. 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 is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. 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	solid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 55 - 59 °C - lit.
Initial boiling point and boiling range	356.5±32.0 °C(Predicted)
Flash point	Not applicable
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	log Pow: 2,078
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

Exposure to light. Exposure to moisture

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

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

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

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

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: Not available

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

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

Harmful to aquatic life.

SECTION 13: Disposal considerations

Waste treatment methods**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

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:

IATA:

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: 1993 IMDG: 1993 IATA: 1993

ADR/RID: 1193 IMDG: 1193 IATA: 1193

ADR/RID: 8 IMDG: 8 IATA: 8

ADR/RID: - IMDG: - IATA: -

ADR/RID: 1707 IMDG: 1707 IATA: 1707

ADR/RID: - IMDG: - IATA: - UN proper shipping name ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 1993 IMDG: 1993 IATA: 1993

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3077 IMDG: 3077 IATA: 3077

UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2,3-Dimethyl- 1,2,3,4-tetrahydroquinoxaline) IMDG:

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2,3-Dimethyl- IATA: Environmentally hazardous substance, solid, n.o.s. tetrahydroquinoxaline)

ADR/RID: FLAMMABLE LIQUID, N.O.S. (1,2-Dichlorobutane) IMDG: FLAMMABLE LIQUID, N.O.S. (1,2-Dichlorobutane) IATA: Flammable liquid, n.o.s. (1,2-Dichlorobutane)

ADR/RID: - IMDG: - IATA: -

ADR/RID: FLAMMABLE LIQUID, N.O.S. (1,1-Dimethoxyhexan) IMDG: FLAMMABLE LIQUID, N.O.S. (1,1-Dimethoxyhexan) IATA: Flammable liquid, n.o.s. (1,1-Dimethoxyhexan)

ADR/RID: III IMDG: III IATA: III

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

ADR/RID: THALLIUM COMPOUND, N.O.S. (Thallic sulphate) IMDG: THALLIUM COMPOUND, N.O.S. (Thallic sulphate) IATA: Thallium compound, n.o.s. (Thallic sulphate)

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

ADR/RID: ETHYL METHYL KETONE IMDG: ETHYL METHYL KETONE IATA: Ethyl methyl ketone

ADR/RID: FLAMMABLE LIQUID, N.O.S. (POMELO ALDEHYDE) IMDG: FLAMMABLE LIQUID, N.O.S. (POMELO ALDEHYDE) IATA: Flammable liquid, n.o.s. (POMELO ALDEHYDE)

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

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

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

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: - IMDG: - IATA: -

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

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

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: no IMDG Marine pollutant: no IATA: no Special precautions for user Further information Not classified as dangerous in the meaning of transport regulations.

ADR/RID: 3 IMDG: 3 IATA: 3

(2,3-Dimethyl-1,2,3,4- ADR/RID: 9 IMDG: 9 IATA: 9

Packaging group

ADR/RID: III IMDG: III IATA: III

ADR/RID: III IMDG: III IATA: III

ADR/RID: III IMDG: III IATA: III

No data available

No data available

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

ADR/RID: II IMDG: II IATA: II

No data available

No data available

ADR/RID: II IMDG: II IATA: II

Environmental hazards

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

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

No data available

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 1,2,3,4-tetrahydroquinoxaline) 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.

Special precautions for user

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

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

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

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

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

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

SECTION 16: Other information

Abbreviations and acronyms

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

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.