

Chemical Safety Data Sheet MSDS / SDS

7-[(1S,2R,3R,4R)-3-[(1E,3R)-3-HYDROXY-4-(4-IODOPHENOXY)-1-BUTENYL]-7-OXABICYCLO[2.2.1]HEPT-2-YL]-5Z-HEPTENOIC ACID

Revision Date:2024-11-23 Revision Number:1

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

Product name : 7-[(1S,2R,3R,4R)-3-[(1E,3R)-3-HYDROXY-4-(4-IODOPHENOXY)-1-BUTENYL]-7-OXABICYCLO[2.2.1]HEPT-2-YL]-5Z-HEPTENOIC ACID

CBnumber : CB7674385

CAS : 128719-90-4

EINECS Number : 200-578-6

Synonyms : I-BOP

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

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

P337+P313 IF eye irritation persists: Get medical advice/attention.

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

Continuerinsing.

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

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H319 Causes serious eye irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 7-[(1S,2R,3R,4R)-3-[(1E,3R)-3-HYDROXY-4-(4-IODOPHENOXY)-1-BUTENYL]-7-OXABICYCLO[2.2.1]HEPT-2-YL]-5Z-HEPTENOIC ACID
Synonyms	: I-BOP
CAS	: 128719-90-4
EC number	: 200-578-6
MF	: C23H29IO5
MW	: 512.38

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material 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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. 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

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen iodide

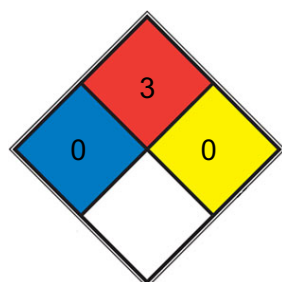
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704



HEALTH 0 Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials

FIRE 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

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

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.

Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

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. 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.

Body Protection

Impervious clothing, Flame retardant antistatic protective 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

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless liquid, clear
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	-144,0 °C
Initial boiling point and boiling range	78,0 - 80,0 °C
Flash point	14,0 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 19 %(V) Lower explosion limit: 3,3 %(V)
Vapour pressure	59,5 hPa at 20,0 °C
Vapour density	No data available
Relative density	0,7974 g/cm ³
Water solubility	completely soluble
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	363,0 °C
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

Heat, flames and sparks.

Incompatible materials

Alkali metals, Ammonia, Oxidizing agents, Peroxides

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen iodide

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

No data available

LD50 Oral - Rat - male and female - 10.470 mg/kg (ethanol) (OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 124,7 mg/l (ethanol) (OECD Test Guideline 403)

Skin corrosion/irritation

No data available

Skin - Rabbit (ethanol)

Result: No skin irritation - 24 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

No data available

Eyes - Rabbit (ethanol)

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

Respiratory or skin sensitization

No data available

Maximization Test - Guinea pig (ethanol)

Result: negative

(OECD Test Guideline 406)

Remarks: (in analogy to similar products)

Germ cell mutagenicity

No data available Ames test (ethanol)

Salmonella typhimurium Result: negative

In vitro mammalian cell gene mutation test (ethanol) mouse lymphoma cells

Result: negative

OECD Test Guideline 478 (ethanol) Mouse - male

Result: Positive results were obtained in some in vivo tests.

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 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

Repeated dose toxicity - Rat - male - Oral - NOAEL (No observed adverse effect level) - 1.730 mg/kg - LOAEL (Lowest observed adverse effect level) - 3.200 mg/kg (ethanol)

RTECS: Not available

irritant effects, respiratory paralysis, Dizziness, narcosis, inebriation, euphoria, Nausea, Vomiting (ethanol)

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

SECTION 12: Ecological information

Toxicity

No data available

Toxicity to fish

flow-through test LC50 - *Pimephales promelas* (fathead minnow) -

15.300 mg/l - 96 h (ethanol) (US-EPA)

Toxicity to daphnia and other aquatic invertebrates

static test LC50 - *Ceriodaphnia dubia* (water flea) - 5.012 mg/l - 48 h (ethanol)

Remarks: (ECHA)

Toxicity to algae

static test ErC50 - *Chlorella vulgaris* (Fresh water algae) - 275 mg/l

- 72 h (ethanol)

(OECD Test Guideline 201)

Toxicity to bacteria

static test IC50 - activated sludge - > 1.000 mg/l - 3 h (ethanol) (OECD Test Guideline 209)

Persistence and degradability

No data available

Biochemical Oxygen Demand (BOD)

Theoretical oxygen demand

930 - 1.670 mg/g (ethanol) Remarks: (Lit.)

2.100 mg/g (ethanol) Remarks: (Lit.)

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

No data available

Additional ecological information

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

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: 1170 IMDG: 1170 IATA: 1170

UN proper shipping name

	ADR/RID: ETHANOL SOLUTION IMDG: ETHANOL SOLUTION	
	IATA: Ethanol solution	
14.3	Transport hazard class(es)	
	ADR/RID: 3 IMDG: 3	IATA: 3
14.4	Packaging group	
	ADR/RID: II IMDG: II	IATA: II
14.5	Environmental hazards	
	ADR/RID: no IMDG Marine pollutant: no	IATA: no
14.6	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

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>
New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>
European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>
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/>
Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>
EC Inventory:Not 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

- 【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.