

SAFETY DATA SHEETS

According to the UN GHS revision 8

Version: 1.0

Creation Date: July 15, 2019

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SECTION 1: Identification

1.1 GHS Product identifier

Product name 1-Octanol

1.2 Other means of identification

Other names

1.3 Recommended use of the chemical and restrictions on use

Identified usesFragrancesUses advised againstno data available

1.4 Supplier's details

Company Target Molecule Corp.

Address Suite 260, 36 Washington Street, Wellesley Hills, Massachusetts, USA

Tel/Fax +1 (857) 239-0968

1.5 Emergency phone number

Emergency phone number 400-821-2233

Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Eye irritation, Category 2

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Warning

Hazard statement(s) H319 Causes serious eye irritation

H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention P264 Wash ... thoroughly after handling.

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

protection/...

P273 Avoid release to the environment.

Response P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove

contact lenses, if present and easy to do. Continue rinsing.

Storage none

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.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Octan-1-ol	Octan-1-ol	111-87-5	203-917-6	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air. rest.

Following skin contact

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. Do NOT induce vomiting. Give one or two glasses of water to drink.

4.2 Most important symptoms/effects, acute and delayed

Irritates skin and eyes. (USCG, 1999)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Higher alcohols (>3 carbons) and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Specific hazards arising from the chemical

Combustible. Above 81°C explosive vapour/air mixtures may be formed.

5.3 Special protective actions for fire-fighters

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

SECTION 6: Accidental release measures

6.1 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 covered containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment.

6.2 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 covered containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment.

6.3 Methods and materials for containment and cleaning up

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. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.; 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 Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations. Keep in suitable, closed containers for disposal.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames. Above 81°C use a closed system and ventilation. 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.

7.2 Conditions for safe storage, including any incompatibilities

Separated from strong oxidants. Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place. Storage class (TRGS 510): Combustible liquids

Recommended storage temperature: Store at -20°C

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

MAK: 54 mg/m3, 10 ppm; peak limitation category: I(1); pregnancy risk group: C

Biological limit values

no data available

8.2 Appropriate engineering controls

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

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state Liquid.

Colour Colourless.

Odour Fresh orange rose odor

Melting point/freezing point -13.5 °C. Atm. press.:Ca. 1 atm.

Boiling point or initial boiling point 194 °C. Atm. press.:Ca. 1 atm. Remarks:Measured: 380.5 °F.

and boiling range

Flammability Combustible.

Lower and upper explosion no data available

limit/flammability limit

Flash point 86.5 °C. Atm. press.:Ca. 101.5 kPa.

Auto-ignition temperature Ca. 294 °C. Atm. press.:Ca. 1 013 mBar.

Decomposition temperature no data available pH no data available

Kinematic viscosity kinematic viscosity (in mm²/s) = 5.584. Temperature:40°C.

Solubility In water, 540 mg/L at 25 deg C

Partition coefficient n- log Pow = 3.5. Temperature:23 °C.

octanol/water

Vapour pressure Ca. 0.764 mBar. Temperature: Ca. 38 °C. Remarks: Measured temperature: 100 °F.

Density and/or relative density 0.828 g/cm³. Temperature:15.56 °C.

Relative vapour density 4.5 (vs air)

Particle characteristics no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Reacts with strong oxidants. Reacts with strong oxidants.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Combustible liquid when exposed to heat or flame...Attacks plastics [Handling Chemicals Safely 1980. p. 236]. Acetyl bromide reacts violently with alcohols or water [Merck 11th ed. 1989]. Mixtures of alcohols with concentrated sulfuric acid and strong hydrogen peroxide can cause explosions. Example: an explosion will occur if dimethylbenzylcarbinol is added to 90% hydrogen peroxide then acidified with concentrated sulfuric acid. Mixtures of ethyl alcohol with concentrated hydrogen peroxide form powerful explosives. Mixtures of hydrogen peroxide and 1-phenyl-2-methyl propyl alcohol tend to explode if acidified with 70% sulfuric acid [Chem. Eng. News 45(43):73. 1967; J, Org. Chem. 28:1893. 1963]. Alkyl hypochlorites are violently explosive. They are readily obtained by reacting hypochlorous acid and alcohols either in aqueous solution or mixed aqueous-carbon tetrachloride solutions. Chlorine plus alcohols would similarly yield alkyl hypochlorites. They decompose in the cold and explode on exposure to sunlight or heat. Tertiary hypochlorites are less unstable than secondary or primary hypochlorites [NFPA 491 M. 1991]. Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence [Wischmeyer 1969].

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Can react with oxidizing materials.

10.6 Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 rat (male/female) > 5 000 mg/kg bw.
- Inhalation: no data available
- Dermal: LD50 rabbit (male/female) 2 000 4 000 mg/kg bw.

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 and respiratory tract. The substance is mildly irritating to the skin. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis.

STOT-repeated exposure

The substance defats the skin, which may cause dryness or cracking.

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

12.1 Toxicity

- Toxicity to fish: LC50 Pimephales promelas 13.3 mg/L 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC0 Daphnia magna 6.8 mg/L 24 h.
- Toxicity to algae: EC50 Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) 6.5 mg/L 48 h.
- Toxicity to microorganisms: TT or EC3 Entosiphon sulcatum 44 mg/L 72 h.

12.2 Persistence and degradability

AEROBIC: A number of aerobic biological screening studies, which utilized settled waste water, sewage, or activated sludge for inocula, have demonstrated that 1-octanol is readily biodegradable(1-9). Five day BOD tests show theoretical BODs of 33(1), 37(2) and 62.4%(3). A ring test involving 14 laboratories found a mean degradation of 85% in 28 day test(4). Biodegradation of 1-octanol was 71% after incubation in the dark at 20 degrees C for 7 days using an inoculation with activated sludge and measuring theoretical carbon dioxide evolved(5). Other screening test data yielded a half-life of 22 hours(SRC) based on a first order biodegradation rate of 0.0313/hr(6) for 1-octanol. 1-Octanol, present at 100 mg/L, reached 89% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(7).

12.3 Bioaccumulative potential

An estimated BCF of 44 was calculated in fish for 1-octanol(SRC), using a log Kow of 3.00(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC).

12.4 Mobility in soil

The Koc of 1-octanol is reported as 38(1). According to a classification scheme(2), this Koc value suggests that 1-octanol is expected to have very high mobility in soil(SRC).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 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

14.1 UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No IMDG: No IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
Octan-1-ol	Octan-1-ol	111-87-5	203-917-6
European Inventory of Existing Commercial Chemical Substances (EINECS)			
EC Inventory			
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			
New Zealand Inventory of Chemicals (NZIoC)			
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			
Korea Existing Chemicals List (KECL)			

SECTION 16: Other information

Information on revision

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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?pageID=0&request_locale=en
- CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- ChemlDplus, 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/

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