

**N-Octyl Mercaptan**

Version 1.21

Revision Date 2021-09-27

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

Product Name : N-Octyl Mercaptan
Material : 1115893, 1086427, 1092079, 1089361, 1086426, 1021507,
1021501, 1021505, 1021503, 1021502, 1021508, 1021506,
1021504, 1024813, 1026777, 1036311, 1021509, 1035162,
1024812, 1033723

Company : Chevron Phillips Chemical Company LP
Specialty Chemicals
10001 Six Pines Drive
The Woodlands, TX 77380

Emergency telephone:**Health:**

866.442.9628 (North America)

1.832.813.4984 (International)

Transport:

CHEMTREC 800.424.9300 or 703.527.3887(int'l)

Asia: CHEMWATCH (+612 9186 1132) China: 0532 8388 9090

EUROPE: BIG +32.14.584545 (phone) or +32.14583516 (telefax)

Mexico CHEMTREC 01-800-681-9531 (24 hours)

South America SOS-Cotec Inside Brazil: 0800.111.767 Outside Brazil: +55.19.3467.1600

Argentina: +(54)-1159839431

Responsible Department : Product Safety and Toxicology Group
E-mail address : SDS@CPChem.com
Website : www.CPChem.com

SECTION 2: Hazards identification**Classification of the substance or mixture**

This product has been classified in accordance with the hazard communication standard 29 CFR 1910.1200; the SDS and labels contain all the information as required by the standard.

Classification

: Flammable liquids, Category 4
Skin sensitization, Category 1

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Labeling

Symbol(s)

:



Signal Word

:

Warning

Hazard Statements

:

H227: Combustible liquid.
H317: May cause an allergic skin reaction.

Precautionary Statements

:

Prevention:
 P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
 P261 Avoid breathing dust/fume/gas/mist/vapors/spray.
 P272 Contaminated work clothing should not be allowed out of the workplace.
 P280 Wear protective gloves/ eye protection/ face protection.
Response:
 P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
 P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
 P363 Wash contaminated clothing before reuse.
 P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
Storage:
 P403 + P235 Store in a well-ventilated place. Keep cool.
Disposal:
 P501 Dispose of contents/ container to an approved waste disposal plant.

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.

NTP

No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

SECTION 3: Composition/information on ingredients

Synonyms

:

1-Octanethiol
normal-Octyl mercaptan
NOM
NC8SH

Molecular formula

:

C₈H₁₈S

Component	CAS-No.	Weight %
n-Octyl Mercaptan	111-88-6	98.5 - 100

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SECTION 4: First aid measures

- General advice : Move out of dangerous area. Show this material safety data sheet to the doctor in attendance. Material may produce a serious, potentially fatal pneumonia if swallowed or vomited.
- If inhaled : If unconscious, place in recovery position and seek medical advice. If symptoms persist, call a physician.
- In case of skin contact : If on skin, rinse well with water. If on clothes, remove clothes.
- In case of eye contact : Flush eyes with water as a precaution. Remove contact lenses. Protect unharmed eye. Keep eye wide open while rinsing. If eye irritation persists, consult a specialist.
- If swallowed : Keep respiratory tract clear. Do NOT induce vomiting. Never give anything by mouth to an unconscious person. If symptoms persist, call a physician. Take victim immediately to hospital.

SECTION 5: Firefighting measures

- Flash point : 69-71°C (156-160°F) at 101.325 kPa
Method: EU Method A.9
- Autoignition temperature : No data available
- Suitable extinguishing media : Carbon dioxide (CO₂).
- Unsuitable extinguishing media : High volume water jet.
- Specific hazards during fire fighting : Do not allow run-off from fire fighting to enter drains or water courses.
- Special protective equipment for fire-fighters : Wear self-contained breathing apparatus for firefighting if necessary.
- Further information : Collect contaminated fire extinguishing water separately. This must not be discharged into drains. Fire residues and contaminated fire extinguishing water must be disposed of in accordance with local regulations. For safety reasons in case of fire, cans should be stored separately in closed containments. Use a water spray to cool fully closed containers.
- Fire and explosion protection : Do not spray on a naked flame or any incandescent material. Keep away from open flames, hot surfaces and sources of ignition.
- Hazardous decomposition products : Carbon oxides. Sulfur oxides.

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SECTION 6: Accidental release measures

- Personal precautions : Use personal protective equipment. Ensure adequate ventilation.
- Environmental precautions : Prevent product from entering drains. Prevent further leakage or spillage if safe to do so. If the product contaminates rivers and lakes or drains inform respective authorities.
- Methods for 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). Keep in suitable, closed containers for disposal.

SECTION 7: Handling and storage**Handling**

- Advice on safe handling : Avoid formation of aerosol. Do not breathe vapors/dust. Avoid exposure - obtain special instructions before use. Avoid contact with skin and eyes. For personal protection see section 8. Smoking, eating and drinking should be prohibited in the application area. Provide sufficient air exchange and/or exhaust in work rooms. Dispose of rinse water in accordance with local and national regulations. Persons susceptible to skin sensitization problems or asthma, allergies, chronic or recurrent respiratory disease should not be employed in any process in which this mixture is being used.
- Advice on protection against fire and explosion : Do not spray on a naked flame or any incandescent material. Keep away from open flames, hot surfaces and sources of ignition.

Storage

- Requirements for storage areas and containers : No smoking. Keep in a well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Observe label precautions. Electrical installations / working materials must comply with the technological safety standards.

SECTION 8: Exposure controls/personal protection**Ingredients with workplace control parameters**

US

Components	Basis	Value	Control parameters	Note
n-Octyl Mercaptan	NIOSH REL	C	0.5 ppm, 3 mg/m ³	

Engineering measures

Adequate ventilation to control airborne concentrations below the exposure guidelines/limits.

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Consider the potential hazards of this material (see Section 2), applicable exposure limits, job activities, and other substances in the work place when designing engineering controls and selecting personal protective equipment. If engineering controls or work practices are not adequate to prevent exposure to harmful levels of this material, the personal protective equipment listed below is recommended. The user should read and understand all instructions and limitations supplied with the equipment since protection is usually provided for a limited time or under certain circumstances.

Personal protective equipment

- Respiratory protection : Wear a supplied-air NIOSH approved respirator unless ventilation or other engineering controls are adequate to maintain minimal oxygen content of 19.5% by volume under normal atmospheric pressure. Wear a NIOSH approved respirator that provides protection when working with this material if exposure to harmful levels of airborne material may occur, such as: Air-Purifying Respirator for Organic Vapors. Use a positive pressure, air-supplying respirator if there is potential for uncontrolled release, aerosolization, exposure levels are not known, or other circumstances where air-purifying respirators may not provide adequate protection.
- Hand protection : The suitability for a specific workplace should be discussed with the producers of the protective gloves. Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. Also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion, and the contact time. Gloves should be discarded and replaced if there is any indication of degradation or chemical breakthrough.
- Eye protection : Eye wash bottle with pure water. Tightly fitting safety goggles.
- Skin and body protection : Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place. Wear as appropriate: Flame retardant protective clothing. Remove and wash contaminated clothing before re-use. Skin should be washed after contact. Footwear protecting against chemicals.
- Hygiene measures : When using do not eat or drink. When using do not smoke. Wash hands before breaks and at the end of workday.

SECTION 9: Physical and chemical properties**Information on basic physical and chemical properties****Appearance**

- Form : liquid
 Physical state : liquid
 Color : Colorless
 Odor : Pungent

Safety data

- Flash point : 69-71°C (156-160°F) at 101.325 kPa
 Method: EU Method A.9

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Lower explosion limit	: No data available
Upper explosion limit	: No data available
Oxidizing properties	: No
Autoignition temperature	: No data available
Molecular formula	: C ₈ H ₁₈ S
Molecular weight	: 146.32 g/mol
pH	: Not applicable
Pour point	: No data available
Boiling point/boiling range	: 199°C (390°F)
Vapor pressure	: 0.02 PSI at 37.8°C (100.0°F)
Relative density	: 0.85 at 16 °C (61 °F)
Water solubility	: negligible
Partition coefficient: n-octanol/water	: No data available
Viscosity, kinematic	: 1.04 mm ² /s at 40°C (104°F)
Relative vapor density	: 1 (Air = 1.0)
Evaporation rate	: No data available

SECTION 10: Stability and reactivity

Reactivity	: Stable under recommended storage conditions.
Chemical stability	: This material is considered stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.
Possibility of hazardous reactions	
Hazardous reactions	: Hazardous reactions: Hazardous polymerization does not occur. Further information: No decomposition if stored and applied as directed.

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	Hazardous reactions: Vapors may form explosive mixture with air.
Conditions to avoid	: Heat, flames and sparks.
Materials to avoid	: May react with oxygen and strong oxidizing agents, such as chlorates, nitrates, peroxides, etc.
Hazardous decomposition products	: Carbon oxides Sulfur oxides
Other data	: No decomposition if stored and applied as directed.

SECTION 11: Toxicological information**Acute oral toxicity**

n-Octyl Mercaptan : LD50: 2,436 mg/kg
Species: Rat
Sex: male and female
Method: Fixed Dose Method

Acute inhalation toxicity

n-Octyl Mercaptan : LC50: > 0.24 mg/l
Exposure time: 4 h
Species: Rat
Sex: male and female
Test atmosphere: vapor
Method: OECD Test Guideline 403
An LC50/inhalation/4h/rat could not be determined because no mortality of rats was observed at the maximum achievable concentration.

Acute dermal toxicity

n-Octyl Mercaptan : LD50: > 1,680 mg/kg
Species: Rat
Sex: male and female
Method: OECD Test Guideline 402

Skin irritation

n-Octyl Mercaptan : slight irritation. largely based on animal evidence.

Eye irritation

n-Octyl Mercaptan : slight irritation. largely based on animal evidence.

Sensitization

n-Octyl Mercaptan : May cause sensitization by skin contact.
largely based on animal evidence.

Repeated dose toxicity

n-Octyl Mercaptan : Species: Rat, males

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Sex: males
Application Route: Oral
Dose: 0, 10, 50, 250 mg/kg
Exposure time: 35 D
Number of exposures: once daily
NOEL: 50 mg/kg
Method: OECD Guideline 422

Species: Rat, females
Sex: females
Application Route: Oral
Dose: 0, 10, 50, 250 mg/kg
Number of exposures: once daily
NOEL: 50 mg/kg
Method: OECD Guideline 422

Genotoxicity in vitro

n-Octyl Mercaptan

: Test Type: Reverse mutation assay
Metabolic activation: with and without metabolic activation
Method: Mutagenicity (Escherichia coli - reverse mutation assay)
Result: negative

Test Type: Chromosome aberration test in vitro
Test system: Human lymphocytes
Metabolic activation: with and without metabolic activation
Result: negative

Test Type: Sister chromatid exchange
Metabolic activation: with and without metabolic activation
Result: negative

Genotoxicity in vivo

n-Octyl Mercaptan

: Test Type: Micronucleus test
Species: Mouse
Method: Mutagenicity (micronucleus test)
Result: negative

Reproductive toxicity

n-Octyl Mercaptan

: Species: Rat
Sex: male
Application Route: Oral diet
Dose: 0, 10, 50, 250 mg/kg
Exposure time: 35 D
Number of exposures: once daily
Method: OECD Guideline 422
NOAEL Parent: 250 mg/kg
NOAEL F1: 250 mg/kg

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Species: Rat
 Sex: female
 Application Route: Oral diet
 Dose: 0, 10, 50, 250 mg/kg
 Number of exposures: once daily
 Method: OECD Guideline 422
 NOAEL Parent: 50 mg/kg
 NOAEL F1: 250 mg/kg

Developmental Toxicity

n-Octyl Mercaptan : Species: Rat
 Application Route: Oral diet
 Dose: 0, 10, 50, 250 mg/kg
 Number of exposures: once daily
 NOAEL Teratogenicity: 250 mg/kg

Aspiration toxicity

n-Octyl Mercaptan : May be harmful if swallowed and enters airways.

CMR effects

n-Octyl Mercaptan : Mutagenicity: Tests on bacterial or mammalian cell cultures did not show mutagenic effects.
 Teratogenicity: Animal testing did not show any effects on fetal development.
 Reproductive toxicity: Animal testing did not show any effects on fertility.

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Further information**

: Solvents may degrease the skin.

SECTION 12: Ecological information**Toxicity to fish**

n-Octyl Mercaptan : LC50: 0.326 mg/l
 Exposure time: 96 h
 Species: *Oryzias latipes* (Orange-red killifish)
 semi-static test Analytical monitoring: yes
 Method: OECD Test Guideline 203
 Very toxic to fish.

Toxicity to daphnia and other aquatic invertebrates

n-Octyl Mercaptan : 0.0243 mg/l
 Exposure time: 48 h
 Species: *Daphnia magna* (Water flea)
 Immobilization Analytical monitoring: yes
 Method: OECD Test Guideline 202
 Very toxic to aquatic organisms.

Toxicity to algae

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n-Octyl Mercaptan : 0.039 mg/l
 Exposure time: 72 h
 Species: Pseudokirchneriella subcapitata (microalgae)
 semi-static test Analytical monitoring: yes
 Method: OECD Test Guideline 201
 Very toxic to algae.

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

n-Octyl Mercaptan : > 0.00467 mg/l
 Exposure time: 21 d
 Species: Daphnia magna (Water flea)
 Toxic effects on fish and plankton

Biodegradability

n-Octyl Mercaptan : Result: Not readily biodegradable.
 0 %
 Testing period: 28 Days
 Method: OECD Test Guideline 301
 Information given is based on data obtained from similar substances.

Bioaccumulation

n-Octyl Mercaptan : Bioconcentration factor (BCF): 11.83
 Method: QSAR modeled data

Mobility

n-Octyl Mercaptan : Medium: Soil
 Method: Calculation, Mackay Level III Fugacity Model
 Content: 47.8 %
 This product may float or sink in water.

: Medium: Water
 Method: Calculation, Mackay Level III Fugacity Model
 Content: 25 %
 This product may float or sink in water.

Additional ecological information : Very toxic to aquatic life with long lasting effects.

Ecotoxicology Assessment**Short-term (acute) aquatic hazard**

n-Octyl Mercaptan : Very toxic to aquatic life.

Long-term (chronic) aquatic hazard

n-Octyl Mercaptan : Very toxic to aquatic life with long lasting effects.

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SECTION 13: Disposal considerations

The information in this SDS pertains only to the product as shipped.

Use material for its intended purpose or recycle if possible. This material, if it must be discarded, may meet the criteria of a hazardous waste as defined by US EPA under RCRA (40 CFR 261) or other State and local regulations. Measurement of certain physical properties and analysis for regulated components may be necessary to make a correct determination. If this material is classified as a hazardous waste, federal law requires disposal at a licensed hazardous waste disposal facility.

- Product : The product should not be allowed to enter drains, water courses or the soil. Do not contaminate ponds, waterways or ditches with chemical or used container. Send to a licensed waste management company.
- Contaminated packaging : Empty remaining contents. Dispose of as unused product. Do not re-use empty containers. Do not burn, or use a cutting torch on, the empty drum.

SECTION 14: Transport information

The shipping descriptions shown here are for bulk shipments only, and may not apply to shipments in non-bulk packages (see regulatory definition).

Consult the appropriate domestic or international mode-specific and quantity-specific Dangerous Goods Regulations for additional shipping description requirements (e.g., technical name or names, etc.) Therefore, the information shown here, may not always agree with the bill of lading shipping description for the material. Flashpoints for the material may vary slightly between the SDS and the bill of lading.

US DOT (UNITED STATES DEPARTMENT OF TRANSPORTATION)

NA1993, COMBUSTIBLE LIQUID, N.O.S., (N-OCTYL MERCAPTAN), III

IMO / IMDG (INTERNATIONAL MARITIME DANGEROUS GOODS)

UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (N-OCTYL MERCAPTAN), 9, III, (69-71°C), MARINE POLLUTANT, (N-OCTYL MERCAPTAN)

IATA (INTERNATIONAL AIR TRANSPORT ASSOCIATION)

UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (N-OCTYL MERCAPTAN), 9, III

ADR (AGREEMENT ON DANGEROUS GOODS BY ROAD (EUROPE))

UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (N-OCTYL MERCAPTAN), 9, III, (-)

RID (REGULATIONS CONCERNING THE INTERNATIONAL TRANSPORT OF DANGEROUS GOODS (EUROPE))

UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (N-OCTYL MERCAPTAN), 9, III

ADN (EUROPEAN AGREEMENT CONCERNING THE INTERNATIONAL CARRIAGE OF DANGEROUS GOODS BY INLAND WATERWAYS)

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UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (N-OCTYL MERCAPTAN), 9, III

Other information	: n-Octyl Mercaptan, S.T. 1, Cat. X
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Maritime transport in bulk according to IMO instruments

SECTION 15: Regulatory information**National legislation**

SARA 311/312 Hazards : Flammable (gases, aerosols, liquids, or solids)
Respiratory or skin sensitization

CERCLA Reportable Quantity : This material does not contain any components with a CERCLA RQ.

SARA 302 Reportable Quantity : This material does not contain any components with a SARA 302 RQ.

SARA 302 Threshold Planning Quantity : This material does not contain any components with a section 302 EHS TPQ.

SARA 304 Reportable Quantity : This material does not contain any components with a section 304 EHS RQ.

SARA 313 Components : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

Ozone-Depletion Potential : This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

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This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

US State Regulations

Pennsylvania Right To Know : n-Octyl Mercaptan - 111-88-6

Pennsylvania Right To Know : n-Octyl Mercaptan - 111-88-6

New Jersey Right To Know : n-Octyl Mercaptan - 111-88-6

California Prop. 65 Components : This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

Europe REACH	:	On the inventory, or in compliance with the inventory
Switzerland CH INV	:	On the inventory, or in compliance with the inventory
United States of America (USA) TSCA	:	On or in compliance with the active portion of the TSCA inventory
Canada DSL	:	All components of this product are on the Canadian DSL
Australia AICS	:	On the inventory, or in compliance with the inventory
New Zealand NZIoC	:	On the inventory, or in compliance with the inventory
Japan ENCS	:	On the inventory, or in compliance with the inventory
Korea KECI	:	All substances in this product were registered, notified to be registered, or exempted from registration by CPChem through an Only Representative according to K-REACH regulations. Importation of this product is permitted if the Korean Importer of Record was included on CPChem's notifications or if the Importer of Record themselves notified the substances.
Philippines PICCS	:	On the inventory, or in compliance with the inventory
China IECSC	:	On the inventory, or in compliance with the inventory
Taiwan TCSI	:	On the inventory, or in compliance with the inventory

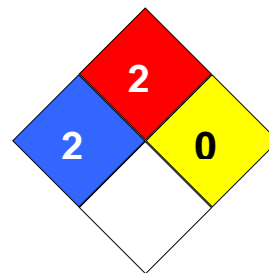
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SECTION 16: Other information

NFPA Classification : Health Hazard: 2
Fire Hazard: 2
Reactivity Hazard: 0

**Further information**

Legacy SDS Number : 76100

Significant changes since the last version are highlighted in the margin. This version replaces all previous versions.

The information in this SDS pertains only to the product as shipped.

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

Key or legend to abbreviations and acronyms used in the safety data sheet			
ACGIH	American Conference of Government Industrial Hygienists	LD50	Lethal Dose 50%
AICS	Australia, Inventory of Chemical Substances	LOAEL	Lowest Observed Adverse Effect Level
DSL	Canada, Domestic Substances List	NFPA	National Fire Protection Agency
NDSL	Canada, Non-Domestic Substances List	NIOSH	National Institute for Occupational Safety & Health
CNS	Central Nervous System	NTP	National Toxicology Program
CAS	Chemical Abstract Service	NZIoC	New Zealand Inventory of Chemicals
EC50	Effective Concentration	NOAEL	No Observable Adverse Effect Level
EC50	Effective Concentration 50%	NOEC	No Observed Effect Concentration
EGEST	EOSCA Generic Exposure Scenario Tool	OSHA	Occupational Safety & Health Administration
EOSCA	European Oilfield Specialty Chemicals Association	PEL	Permissible Exposure Limit
EINECS	European Inventory of Existing Chemical Substances	PICCS	Philippines Inventory of Commercial Chemical Substances
MAK	Germany Maximum Concentration Values	PRNT	Presumed Not Toxic
GHS	Globally Harmonized System	RCRA	Resource Conservation Recovery Act
>=	Greater Than or Equal To	STEL	Short-term Exposure Limit
IC50	Inhibition Concentration 50%	SARA	Superfund Amendments and Reauthorization Act.
IARC	International Agency for Research on Cancer	TLV	Threshold Limit Value
IECSC	Inventory of Existing Chemical Substances in China	TWA	Time Weighted Average
ENCS	Japan, Inventory of Existing and	TSCA	Toxic Substance Control Act

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	New Chemical Substances		
KECI	Korea, Existing Chemical Inventory	UVCB	Unknown or Variable Composition, Complex Reaction Products, and Biological Materials
<=	Less Than or Equal To	WHMIS	Workplace Hazardous Materials Information System
LC50	Lethal Concentration 50%		