

AlphaPlus® 1-HEXENE

Version 1.18

Revision Date 2023-11-28

according to GB/T 16483 and GB/T 17519

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

Product Name : AlphaPlus® 1-HEXENE
Material : 1128498, 1117427, 1088135, 1081271, 1084562, 1070002,
1025308, 1017828, 1032321, 1017829, 1028630, 1026835,
1028342, 1011442, 1026834, 1015415

Company : Chevron Phillips Chemical Company LP
Normal Alpha Olefins (NAO)
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

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

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

Austria: VIZ +43 1 406 43 43 (24 hours/day, 7 days/week)

Belgium: 070 245 245 (24 hours/day, 7 days/week)

Bulgaria: +359 2 9154 233

Croatia: +3851 2348 342 (24 hours/day, 7 days/week)

Cyprus: 1401

Czech Republic: Toxicological Information Center +420 224 919 293, +420 224 915 402

Denmark: Danish Poison Center (Giftlinjen): +45 8212 1212

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

Finland: 0800 147 111 09 471 977 (24 hours/day)

France: ORFILA number (INRS): + 33 (0) 1 45 42 59 59 (24 hours/day, 7 days/week)

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

Greece: (0030) 2107793777 (24 hours/day, 7 days/week)

Hungary: +36-80-201-199 (24 hours/day, 7 days/week)

Iceland: 543 2222 (24 hours/day, 7 days/week)

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

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

Latvia: State Fire and Rescue Service, phone number: 112; Toxicology and Sepsis Clinic

Poisoning and Drug Information Center, Hipokrāta 2, Riga, Latvia, LV-1038, phone number +371 67042473. (24 hours.)

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Liechtenstein: BIG +32.14.584545 (phone) or +32.14583516 (telefax)
 Lithuania: +370 (85) 2362052
 Luxembourg: (+352) 8002 5500 (24 hours/day, 7 days/week)
 Malta: +356 2395 2000
 The Netherlands: NVIC: +31 (0)88 755 8000
 Norway: 22 59 13 00 (24 hours/day, 7 days/week)
 Poland: BIG +32.14.584545 (phone) or +32.14583516 (telefax)
 Portugal: CIAV phone number: +351 800 250 250
 Romania: +40213183606
 Slovakia: +421 2 5477 4166
 Slovenia: Phone number: 112
 Spain: National Emergency Telephone Number of Spanish Poison Centre: +34 91 562 04 20 (24 hours/day, 7 days/week)
 Sweden: 112 – ask for Poisons Information

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**

GHS Classification and Labeling: Follow GB 13690, GB 15258 and GB 30000.2 to GB 30000.29 (GHS 2011)

Emergency Overview**Danger**

Form: liquid **Physical state:** liquid **Color:** Clear, colorless **Odor:** No information available.

Hazards : Highly flammable liquid and vapor. May cause respiratory irritation., May cause drowsiness or dizziness. May be fatal if swallowed and enters airways. Toxic to aquatic life. Toxic to aquatic life with long lasting effects.

Classification

: Flammable liquids, Category 2
 Specific target organ toxicity - single exposure, Category 3,
 respiratory tract irritation, Narcotic effects
 Aspiration hazard, Category 1
 Short-term (acute) aquatic hazard, Category 2
 Long-term (chronic) aquatic hazard, Category 2

Labeling

Symbol(s)



Signal Word

: Danger

Hazard Statements

: H225: Highly flammable liquid and vapor.
 H304: May be fatal if swallowed and enters airways.
 H335: May cause respiratory irritation.

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H336: May cause drowsiness or dizziness.
H411: Toxic to aquatic life with long lasting effects.

Precautionary Statements : **Prevention:**
 P210: Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
 P233: Keep container tightly closed.
 P240: Ground/bond container and receiving equipment.
 P241: Use explosion-proof electrical/ ventilating/ lighting/ equipment.
 P242: Use only non-sparking tools.
 P243: Take precautionary measures against static discharge.
 P261: Avoid breathing dust/fume/gas/mist/vapors/spray.
 P271: Use only outdoors or in a well-ventilated area.
 P273: Avoid release to the environment.
 P280: Wear protective gloves/ eye protection/ face protection.

Response:
 P301+P310: IF SWALLOWED: Immediately call a POISON CENTER/doctor.
 P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
 P304 + P340 + P312: IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
 P331: Do NOT induce vomiting.
 P370+P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
 P391: Collect spillage.

Storage:
 P403 + P233: Store in a well-ventilated place. Keep container tightly closed.
 P403 + P235: Store in a well-ventilated place. Keep cool.
 P405: Store locked up.

Disposal:
 P501: Dispose of contents/ container to an approved waste disposal plant.

SECTION 3: Composition/information on ingredients

Synonyms : alpha-Hexene
 Hexene-1
 Hex-1-ene
 Hexylene
 NAO 6
 Butyl Ethylene
 C₆H₁₂

Molecular formula : C₆H₁₂

Chemical name	CAS-No. / EINECS-No.	Concentration [wt%]
1-Hexene	592-41-6	99 - 100
2-Ethyl-1-Butene	760-21-4	0 - 1

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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. Do not give milk or alcoholic beverages. 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 : -26°C (-15°F)
Method: closed cup
- Autoignition temperature : 272°C (522°F)
- Suitable extinguishing media : Alcohol-resistant foam. Carbon dioxide (CO₂). Dry chemical.
- 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. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapors). Use only explosion-proof equipment. Keep away from open flames, hot surfaces and sources of ignition.

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SECTION 6: Accidental release measures

- Personal precautions : Use personal protective equipment. 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.
- 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).

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. Take precautionary measures against static discharges. Provide sufficient air exchange and/or exhaust in work rooms. Container may be opened only under exhaust ventilation hood. Open drum carefully as content may be under pressure. Dispose of rinse water in accordance with local and national regulations.
- Advice on protection against fire and explosion : Do not spray on a naked flame or any incandescent material. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapors). Use only explosion-proof equipment. Keep away from open flames, hot surfaces and sources of ignition.

Storage

- Requirements for storage areas and containers : No smoking. 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. Observe label precautions. Electrical installations / working materials must comply with the technological safety standards.

SECTION 8: Exposure controls/personal protection

Not applicable

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 : If ventilation or other engineering controls are not adequate to maintain minimal oxygen content of 19.5% by volume under normal atmospheric pressure, a supplied-air NIOSH approved respirator may be appropriate. If exposure to harmful levels of airborne material may occur, a NIOSH approved respirator that provides protection may be appropriate, such as: Air-Purifying Respirator for Organic Vapors. A positive pressure, air-supplying respirator may be appropriate 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 antistatic protective clothing. Workers should wear antistatic footwear.
- 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 : Clear, colorless
- Odor : No information available.
- Odor Threshold : No data available

Safety data

- Flash point : -26°C (-15°F)
Method: closed cup

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Lower explosion limit	: 2 %(V)
Upper explosion limit	: 7 %(V)
Flammability (solid, gas)	:
Oxidizing properties	: no
Autoignition temperature	: 272°C (522°F)
Thermal decomposition	: No data available
Molecular formula	: C ₆ H ₁₂
Molecular weight	: 84.18 g/mol
pH	: Not applicable
Pour point	: No data available
Melting point/freezing point	-140°C (-220°F)
Boiling point/boiling range	: 63.5°C (146.3°F)
Vapor pressure	: 176.00 MMHG at 24°C (75°F) 106.30 kPa at 65°C (149°F)
Relative density	: 0.68 at 15 °C (59 °F)
Density	: 645 kg/m ³ at 50°C (122°F) 678 kg/m ³ at 15°C (59°F) 674 g/cm ³ at 20°C (68°F)
Water solubility	: 47 MG/L at 20°C (68°F) slightly soluble
Partition coefficient: n-octanol/water	: log Pow: 3.87
Viscosity, kinematic	: 0.34 cSt at 40°C (104°F)
Relative vapor density	: 2.9 (Air = 1.0)
Evaporation rate	: No data available

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Percent volatile : > 99 %

Conductivity : 4.1 pSm
Method: ASTM D4308

SECTION 10: Stability and reactivity

Reactivity : Stable at normal ambient temperature and pressure.

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 : Further information: No decomposition if stored and applied as directed.

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.

Thermal decomposition : No data available

Other data : No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

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Acute oral toxicity : LD50: > 5,600 mg/kg
Species: Rat
Sex: male and female
Method: Acute toxicity estimate

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Acute inhalation toxicity : No data available

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Acute dermal toxicity : LD50 Dermal: > 3,500 mg/kg
Species: Rabbit
Method: Acute toxicity estimate

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- Skin irritation** : No skin irritation. Repeated or prolonged contact with the mixture may cause removal of natural fat from the skin resulting in desiccation of the skin.
- AlphaPlus® 1-HEXENE**
Eye irritation : No eye irritation.
- AlphaPlus® 1-HEXENE**
Sensitization : Did not cause sensitization on laboratory animals. Information refers to the main ingredient.
- Repeated dose toxicity**
- 1-Hexene : Species: Rat, male
Sex: male
Application Route: oral gavage
Dose: 0, 10, 101, 1010, 3365 mg/kg
Exposure time: 28 day
Number of exposures: daily
NOEL: 101 mg/kg
Lowest observable effect level: 1,010 mg/kg
Test substance: yes
Method: OECD Test Guideline 407
- Species: Rat, female
Sex: female
Application Route: oral gavage
Dose: 0, 10, 101, 1010, 3365 mg/kg
Exposure time: 28 day
Number of exposures: daily
NOEL: 1,010 mg/kg
Lowest observable effect level: 3,365 mg/kg
Test substance: yes
Method: OECD Test Guideline 407
- Species: Rat
Application Route: Inhalation
Dose: 0, 300, 1000, 3000 ppm
Exposure time: 90 day
Number of exposures: 6 h/d, 5 d/wk, 13 wk
NOEL: 3000 ppm
Test substance: yes
- Genotoxicity in vitro**
- 1-Hexene : Test Type: Ames test
Metabolic activation: with and without metabolic activation
Method: Mutagenicity (Escherichia coli - reverse mutation assay)
Result: negative

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Test Type: Unscheduled DNA synthesis assay
Result: negative

Test Type: Mouse lymphoma assay
Result: negative

Test Type: Chromosome aberration test in vitro
Method: OECD Guideline 473
Result: negative

Genotoxicity in vivo

1-Hexene : Test Type: Mouse micronucleus assay
Species: Mouse
Method: Mutagenicity (micronucleus test)
Result: negative

Reproductive toxicity

1-Hexene : Species: Rat
Sex: males
Application Route: oral gavage
Dose: 0, 100, 500, 1000 mg/kg
Number of exposures: daily
Test period: 44 d
Test substance: yes
Method: OECD Guideline 421
NOAEL Parent: 1,000 mg/kg
NOAEL F1: 1,000 mg/kg

Species: Rat
Sex: females
Application Route: oral gavage
Dose: 0, 100, 500, 1000 mg/kg
Number of exposures: daily
Test period: 41-51 d
Test substance: yes
Method: OECD Guideline 421
NOAEL Parent: 1,000 mg/kg
NOAEL F1: 1,000 mg/kg

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Aspiration toxicity**

: May be fatal if swallowed and enters airways.

CMR effects

1-Hexene : Carcinogenicity: Not available
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.

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

1-Hexene : LC50: 5.6 mg/l
Exposure time: 96 h
Species: Oncorhynchus mykiss (rainbow trout)
semi-static test Test substance: yes
Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

1-Hexene : EC50: 4.4 mg/l
Exposure time: 48 h
Species: Daphnia magna (Water flea)
static test Test substance: no
Method: OECD Test Guideline 202
Information given is based on data obtained from similar substances.

Toxicity to algae

1-Hexene : NOEC: 1.8 mg/l
Exposure time: 96 h
Species: Pseudokirchneriella subcapitata (green algae)
Growth inhibition Method: OECD Test Guideline 201
Information given is based on data obtained from similar substances.

EC50: > 5.5 mg/l
Exposure time: 96 h
Species: Pseudokirchneriella subcapitata (green algae)
Growth inhibition Method: OECD Test Guideline 201
Information given is based on data obtained from similar substances.

Biodegradability : This material is expected to be readily biodegradable.

Elimination information (persistence and degradability)

Bioaccumulation : This material is not expected to bioaccumulate.

Mobility : No data available

Results of PBT assessment

1-Hexene : Non-classified PBT substance, Non-classified vPvB substance

Additional ecological information : An environmental hazard cannot be excluded in the event of unprofessional handling or disposal., Toxic to aquatic life.

Ecotoxicology Assessment

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Short-term (acute) aquatic hazard : Toxic to aquatic life.
Long-term (chronic) aquatic hazard : No data available

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)

UN2370, 1-HEXENE, 3, II

IMO / IMDG (INTERNATIONAL MARITIME DANGEROUS GOODS)

UN2370, 1-HEXENE, 3, II, (-26 °C c.c.)

IATA (INTERNATIONAL AIR TRANSPORT ASSOCIATION)

UN2370, 1-HEXENE, 3, II

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

UN2370, 1-HEXENE, 3, II, (D/E)

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

33, UN2370, 1-HEXENE, 3, II

ADN (EUROPEAN AGREEMENT CONCERNING THE INTERNATIONAL CARRIAGE)

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OF DANGEROUS GOODS BY INLAND WATERWAYS)

UN2370, 1-HEXENE, 3, II, ENVIRONMENTALLY HAZARDOUS, (1-HEXENE)

For Tank Vessels and/or Barges:

UN2370, 1-HEXENE, 3, (N3), II, ENVIRONMENTALLY HAZARDOUS, (1-Hexene)

Other information	: Hexene (all isomers), S.T.3., Cat. Y
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Maritime transport in bulk according to IMO instruments

SECTION 15: Regulatory information**Notification status**

Europe REACH	:	This product is in full compliance according to REACH regulation 1907/2006/EC.
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 AIIC	:	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
Philippines PICCS	:	On the inventory, or in compliance with the inventory
Taiwan TCSI	:	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.
China IECSC	:	On the inventory, or in compliance with the inventory

Other regulations	:	Law on the Prevention and Control of Occupational Diseases
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SECTION 16: Other information**Further information**

Legacy SDS Number : PE0016

None.

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

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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%
AIRC	Australian Inventory of Industrial Chemicals	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 New Chemical Substances	TSCA	Toxic Substance Control Act
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%	ATE	Acute toxicity estimate