



# 1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE

## Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 12/09/2014

Revision date:

Version: 1.0

**ECN-2668**

### SECTION 1: Identification of the substance/mixture and of the company/undertaking

#### 1.1. Product identifier

Product form : Mixtures  
Product name. : 1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE  
Product code : ECN-2668

#### 1.2. Relevant identified uses of the substance or mixture and uses advised against

##### 1.2.1. Relevant identified uses

Industrial/Professional use spec : For professional use only.

##### 1.2.2. Uses advised against

No additional information available

#### 1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.  
50 Frontage Road  
Andover, MA 01810  
USA

USA: 1-800-322-1174 Int: 1-978-749-8000  
[cilsales@isotope.com](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

#### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)  
International: 1-202-483-7616 (24 hours)

### SECTION 2: Hazards identification

#### 2.1. Classification of the substance or mixture

##### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Flam. Liq. 3	H226
Acute Tox. 4 (Inhalation)	H332
Skin Irrit. 2	H315
Eye Irrit. 2	H319
STOT SE 3	H336
Asp. Tox. 1	H304

Full text of H-phrases: see section 16

##### Classification according to Directive 67/548/EEC or 1999/45/EC

Xn; R20  
Xn; R65  
R10

Full text of R-phrases: see section 16

##### Classification (GHS-US)

Flam. Liq. 3	H226
Acute Tox. 4 (Inhalation)	H332
Skin Irrit. 2	H315
Eye Irrit. 2A	H319
STOT SE 3	H336
Asp. Tox. 1	H304

##### Adverse physicochemical, human health and environmental effects

Central Nervous System.

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### 2.2. Label elements

#### Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS02

GHS07

GHS08

Signal word (CLP) :

Danger

Hazard statements (CLP) :

H226 - Flammable liquid and vapor  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H332 - Harmful if inhaled  
H336 - May cause drowsiness or dizziness

Precautionary statements (CLP) :

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
P233 - Keep container tightly closed  
P240 - Ground/bond container and receiving equipment  
P241 - Use explosion-proof electrical, lighting, ventilating equipment  
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors  
P264 - Wash Both hands thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear eye protection, face protection, protective clothing, protective gloves

#### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS02

GHS07

GHS08

Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H226 - Flammable liquid and vapor  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H332 - Harmful if inhaled  
H336 - May cause drowsiness or dizziness

Precautionary statements (GHS-US) :

P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking  
P233 - Keep container tightly closed  
P240 - Ground/bond container and receiving equipment  
P241 - Use explosion-proof electrical, lighting, ventilating equipment  
P242 - Use only non-sparking tools  
P243 - Take precautionary measures against static discharge  
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors  
P264 - Wash Both hands thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear eye protection, face protection, protective clothing, protective gloves  
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
P302+P352 - IF ON SKIN: Wash with plenty of soap and water  
P303+P361+P353 - IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower  
P304+P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a POISON CENTER/doctor/physician if you feel unwell  
P331 - If swallowed, do NOT induce vomiting  
P332+P313 - If skin irritation occurs: Get medical advice/attention  
P337+P313 - If eye irritation persists: Get medical advice/attention  
P362 - Take off contaminated clothing and wash before reuse  
P370+P378 - In case of fire: Use Alcohol resistant foam., Carbon dioxide., Dry chemical. for extinction  
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  
P501 - Dispose of contents/container to Comply with applicable regulations.

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### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

Not applicable

### 3.2. Mixtures

Name	Product identifier	%	Classification according to Directive 67/548/EEC
N-NONANE UNLABELED	(CAS No) 111-84-2 (Unlabeled) (EC no) 203-913-4	99.9861	R10 Xn; R20 Xn; R65 R67
1,2,3,4,5,6-HEXACN UNLABELED	(CAS No) 58877-88-6	0.0139	Xn; R22 Xi; R41 Xi; R38 N; R50/53 R48

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
N-NONANE UNLABELED	(CAS No) 111-84-2 (Unlabeled) (EC no) 203-913-4	99.9861	Flam. Liq. 3, H226 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H336 Asp. Tox. 1, H304
1,2,3,4,5,6-HEXACN UNLABELED	(CAS No) 58877-88-6	0.0139	Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Dam. 1, H318 STOT RE 2, H373 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Name	Product identifier	%	Classification (GHS-US)
N-NONANE UNLABELED	(CAS No) 111-84-2 (Unlabeled)	99.9861	Flam. Liq. 3, H226 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H336 Asp. Tox. 1, H304

Full text of R-, H- and EUH-phrases: see section 16

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general	: Move out of dangerous area. Consult a physician and show this safety data sheet.
First-aid measures after inhalation	: Remove to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER/doctor/physician if you feel unwell.
First-aid measures after skin contact	: Remove/Take off immediately all contaminated clothing. Wash with plenty of soap and water. Wash contaminated clothing before reuse.
First-aid measures after eye contact	: Immediately flush eyes with plenty of water for at least 15 minutes. Get immediate medical attention.
First-aid measures after ingestion	: Immediately call a POISON CENTER or doctor/physician.

### 4.2. Most important symptoms and effects, both acute and delayed

Symptoms/injuries after inhalation	: May cause drowsiness or dizziness.
Symptoms/injuries after skin contact	: Causes skin irritation.
Symptoms/injuries after eye contact	: Causes eye irritation.
Symptoms/injuries after ingestion	: May be fatal if swallowed and enters airways.

### 4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

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### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

suitable extinguishing media : For small fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

#### 5.2. Special hazards arising from the substance or mixture

Fire hazard : Flammable liquid and vapor.  
Explosion hazard : May form flammable/explosive vapor-air mixture.  
Reactivity : Vapors may form explosive mixture with air.

#### 5.3. Advice for firefighters

Firefighting instructions : Use water spray to cool unopened containers.  
Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

General measures : Remove ignition sources. Use special care to avoid static electric charges. No naked lights. No smoking.

##### 6.1.1. For non-emergency personnel

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 vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

##### 6.1.2. For emergency responders

No additional information available

#### 6.2. Environmental precautions

Prevent entry to sewers and public waters.

#### 6.3. Methods and material for containment and cleaning up

For containment : Contain spillage, then collect with non-combustible absorbent material. Disposal should be in accordance with applicable Federal, State and local regulations.

#### 6.4. Reference to other sections

No additional information available

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.  
Precautions for safe handling : No naked lights. No smoking. Take precautionary measures against static discharge. Use only non-sparking tools. Use only outdoors or in a well-ventilated area.  
Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Proper grounding procedures to avoid static electricity should be followed. Ground/bond container and receiving equipment. Use explosion-proof electrical equipment.  
Storage conditions : Store at room temperature away from light and moisture.  
Incompatible materials : Heat sources.

#### 7.3. Specific end use(s)

No additional information available

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE		
Italy - Portugal - USA ACGIH	ACGIH TWA (ppm)	200.000000000 ppm Central Nervous System impairment.
N-NONANE UNLABELED (111-84-2 (Unlabeled))		
Italy - Portugal - USA ACGIH	ACGIH TWA (ppm)	200.000000000 ppm Central Nervous System impairment.

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### 8.2. Exposure controls

Personal protective equipment : Protective clothing. Protective goggles. Self-contained breathing apparatus. Gloves.



Hand protection : protective gloves.

Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.

Skin and body protection : Wear suitable protective clothing.

Respiratory protection : Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. Wear respiratory protection.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

*The properties listed below are for the solvent, the main component of this mixture.*

Physical state	: Liquid
Appearance	: Liquid.
Molecular mass	: 334.8
Color	: No data available.
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Melting point	: -53 °C (- 63 °F) - lit
Freezing point	: No data available
Boiling point	: 151 °C (304 °F) - lit
Flash point	: 31.0 °C (87.8 °F) - closed cup
Self ignition temperature	: 205 °C (401 °F)
Decomposition temperature	: No data available
Flammability (solid, gas)	: Flammable liquid and vapor
Vapor pressure	: 12.4 hPa (9.3 mmHg) at 37.7 °C (99.9 °F)
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Solubility	: Water: 0 %
Log Pow	: 5.65
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosive limits	: 0.87 - 2.9 % (V)

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Vapors may form explosive mixture with air.

### 10.2. Chemical stability

See storage and expiration date on CoA.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

Open flame. Overheating. Direct sunlight. Heat. Sparks.

### 10.5. Incompatible materials

Strong oxidizing agents.

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### 10.6. Hazardous decomposition products

May release flammable gases.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Harmful if inhaled.

1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE	
LC50 inhalation rat (ppm)	3200 ppm/4h
ATE (gases)	4500.000 ppmV/4h
ATE (vapors)	11.000 mg/l/4h
ATE (dust, mist)	1.500 mg/l/4h

N-NONANE UNLABELED (111-84-2 (Unlabeled))	
LC50 inhalation rat (ppm)	3200 ppm/4h
ATE (dust, mist)	1.500 mg/l/4h

1,2,3,4,5,6-HEXACN UNLABELED (58877-88-6)	
ATE (oral)	500.000 mg/kg body weight

Skin corrosion/irritation	: Causes skin irritation. Skin - rat - Skin irritation - Draize test
Serious eye damage/irritation	: Causes serious eye irritation. No data available
Respiratory or skin sensitization	: Not available No data available
Germ cell mutagenicity	: Not available
Carcinogenicity	: Not classified
Reproductive toxicity	: Not available
Specific target organ toxicity (single exposure)	: May cause drowsiness or dizziness. May cause drowsiness or dizziness.
Specific target organ toxicity (repeated exposure)	: Not classified No data available
Aspiration hazard	: May be fatal if swallowed and enters airways.
Potential Adverse human health effects and symptoms	: The chemical, physical, and toxicological properties have not been thoroughly investigated.
Symptoms/injuries after inhalation	: May cause drowsiness or dizziness.
Symptoms/injuries after skin contact	: Causes skin irritation.
Symptoms/injuries after eye contact	: Causes eye irritation.
Symptoms/injuries after ingestion	: May be fatal if swallowed and enters airways.

## SECTION 12: Ecological information

### 12.1. Toxicity

No additional information available

### 12.2. Persistence and degradability

1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE	
Persistence and degradability	Not available.

N-NONANE UNLABELED (111-84-2 (Unlabeled))	
Persistence and degradability	Not available.

1,2,3,4,5,6-HEXACN UNLABELED (58877-88-6)	
Persistence and degradability	Not available.

### 12.3. Bioaccumulative potential

1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE	
Log Pow	5.65
Bioaccumulative potential	Indication of bioaccumulation.

# 1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE ECN-2668

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N-NONANE UNLABELED (111-84-2 (Unlabeled))	
Log Pow	5.65
Bioaccumulative potential	Indication of bioaccumulation.

1,2,3,4,5,6-HEXACN UNLABELED (58877-88-6)	
Bioaccumulative potential	Not available.

### 12.4. Mobility in soil

1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE	
Ecology - soil	Not available.

N-NONANE UNLABELED (111-84-2 (Unlabeled))	
Ecology - soil	Not available.

1,2,3,4,5,6-HEXACN UNLABELED (58877-88-6)	
Ecology - soil	Not available.

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Other adverse effects

Other adverse effects : An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.

Waste disposal recommendations : Dispose of contents/container to Comply with applicable regulations.

Additional information : Handle empty containers with care because residual vapors are flammable.

Ecology - waste materials : Hazardous waste due to toxicity.

## SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

### 14.1. UN number

UN-No.(DOT) : 1920  
DOT NA no. UN1920

### 14.2. UN proper shipping name

DOT Proper Shipping Name : Nonanes

Department of Transportation (DOT) Hazard Classes : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120

Hazard labels (DOT) : 3 - Flammable liquid



Packing group (DOT) : III - Minor Danger

DOT Special Provisions (49 CFR 172.102) : B1 - If the material has a flash point at or above 38 C (100 F) and below 93 C (200 F), then the bulk packaging requirements of 173.241 of this subchapter are applicable. If the material has a flash point of less than 38 C (100 F), then the bulk packaging requirements of 173.242 of this subchapter are applicable.  
IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).  
T2 - 1.5 178.274(d)(2) Normal..... 178.275(d)(3)  
TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = 97 / 1 + a (tr - tf) Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.

DOT Packaging Exceptions (49 CFR 173.xxx) : 150

DOT Packaging Non Bulk (49 CFR 173.xxx) : 203

DOT Packaging Bulk (49 CFR 173.xxx) : 242

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### 14.3. Additional information

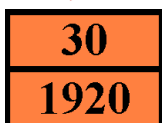
Other information : No supplementary information available.

#### Overland transport

Packing group (ADR) : III  
Class (ADR) : 3 - Flammable liquid  
Hazard identification number (Kemler No.) : 30  
Classification code (ADR) : F1  
Danger labels (ADR) : 3 - Flammable liquids



Orange plates :



Tunnel restriction code : D/E  
Limited quantities (ADR) : 5L  
EAC : 3Y  
Excepted quantities (ADR) : E1

#### Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

MFAG-No : 128

#### Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 60 L

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 220 L

Civil Aeronautics Law : Flammable liquids

### 14.4. Environmental hazards

Other information : No supplementary information available.

### 14.5. Special precautions for user

### 14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

#### 1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard
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#### N-NONANE UNLABELED (111-84-2 (Unlabeled))

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard
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### 15.2. International regulations

#### CANADA

#### 1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE

Listed on the Canadian DSL (Domestic Substances List) inventory.



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### 15.2.1. National regulations

No additional information available

### 15.3. US State regulations

#### 1,2,3,4,5,6-HEXACN (PCN-63) UNLABELED 100 UG/ML IN NONANE()

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.
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#### N-NONANE UNLABELED (111-84-2 (Unlabeled))

U.S. - Massachusetts - Right To Know List  
U.S. - Pennsylvania - RTK (Right to Know) List  
U.S. - New Jersey - Right to Know Hazardous Substance List  
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

## SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of R-, H- and EUH-phrases::

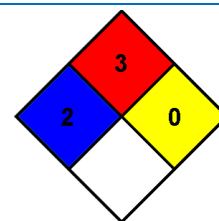
Acute Tox. 4 (Inhalation)	Acute toxicity (inhalation) Category 4
Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Aquatic Acute 1	Hazardous to the aquatic environment - Acute Hazard Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment - Chronic Hazard Category 1
Asp. Tox. 1	Aspiration hazard Category 1
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Eye Irrit. 2	Serious eye damage/eye irritation Category 2
Flam. Liq. 3	Flammable liquids Category 3
Skin Irrit. 2	skin corrosion/irritation Category 2
STOT RE 2	Specific target organ toxicity (repeated exposure) Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H226	Flammable liquid and vapor
H302	Harmful if swallowed
H304	May be fatal if swallowed and enters airways
H315	Causes skin irritation
H318	Causes serious eye damage
H319	Causes serious eye irritation
H332	Harmful if inhaled
H336	May cause drowsiness or dizziness
H373	May cause damage to organs through prolonged or repeated exposure
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects
R10	Flammable
R20	Harmful by inhalation
R22	Harmful if swallowed
R38	Irritating to skin
R41	Risk of serious damage to eyes
R48	Danger of serious damage to health by prolonged exposure
R50/53	Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment
R65	Harmful: may cause lung damage if swallowed
R67	Vapors may cause drowsiness and dizziness
N	Dangerous for the environment
Xi	Irritant
Xn	Harmful

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NFPA health hazard	: 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.
NFPA fire hazard	: 3 - Liquids and solids that can be ignited under almost all ambient conditions.
NFPA reactivity	: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



### HMIS III Rating

Health	: 2 Moderate Hazard - Temporary or minor injury may occur
Flammability	: 3 Serious Hazard
Physical	: 0 Minimal Hazard

### CIL Mixture SDS

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product*