



# 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOCTANE

## 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: 14/11/2014

Revision date:

Version: 1.0

**ECN-5267**

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

### 1.1. Product identifier

Product form : Mixtures  
Product name. : 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOCTANE  
Product code : ECN-5267

### 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. 1	H224
Skin Irrit. 2	H315
STOT SE 3	H336
Asp. Tox. 1	H304
Aquatic Acute 1	H400
Aquatic Chronic 1	H410

Full text of H-phrases: see section 16

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

F; R11  
Xi; R38  
N; R50/53  
R67

Full text of R-phrases: see section 16

#### Classification (GHS-US)

Flam. Liq. 1	H224
Skin Irrit. 2	H315
STOT SE 3	H336
Asp. Tox. 1	H304
Aquatic Acute 1	H400
Aquatic Chronic 1	H410

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

Liver, Kidney.

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ECN-5267

## 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

### 2.2. Label elements

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

Hazard pictograms (CLP)



Signal word (CLP)

: Danger

Hazard statements (CLP)

: H224 - Extremely flammable liquid and vapor  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H336 - May cause drowsiness or dizziness  
H410 - Very toxic to aquatic life with long lasting effects

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, spray, vapors, mist  
P264 - Wash both hands thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P273 - Avoid release to the environment

#### GHS-US labeling

Hazard pictograms (GHS-US)



Signal word (GHS-US)

: Danger

Hazard statements (GHS-US)

: H224 - Extremely flammable liquid and vapor  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H336 - May cause drowsiness or dizziness  
H400 - Very toxic to aquatic life  
H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS-US)

: P210 - Keep away from sparks, open flames, hot surfaces, heat. - No smoking  
P233 - Keep container tightly closed  
P240 - Ground/bond container and receiving equipment  
P241 - Use explosion-proof ventilating, lighting, electrical equipment  
P242 - Use only non-sparking tools  
P243 - Take precautionary measures against static discharge  
P261 - Avoid breathing vapors, spray, mist, gas, fume, dust  
P264 - Wash Both hands thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P273 - Avoid release to the environment  
P280 - Wear protective gloves, protective clothing  
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  
P312 - Call a POISON CENTER/doctor/physician if you feel unwell  
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)  
P331 - If swallowed, do NOT induce vomiting  
P332+P313 - If skin irritation occurs: 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., Water spray for extinction  
P391 - Collect spillage  
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.

# 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

ECN-5267

## 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

### 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
ISOOCTANE UNLABELED	(CAS No)540-84-1 (EC no)208-759-1 (EC index no)601-009-00-8	99.9986	F; R11 Xi; R38 N; R50/53 R67
1,2,3,4,5,8-HEXACN (13C10, 99%)	(CAS No)103426-93-3 (Unlabeled)	0.0014	Xn; R22 Xi; R41 Xi; R36/37 N; R51/53

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
ISOOCTANE UNLABELED	(CAS No)540-84-1 (EC no)208-759-1 (EC index no)601-009-00-8	99.9986	Flam. Liq. 2, H225 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410
1,2,3,4,5,8-HEXACN (13C10, 99%)	(CAS No)103426-93-3 (Unlabeled)	0.0014	Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Dam. 1, H318 STOT SE 3, H335 Aquatic Chronic 2, H411

Name	Product identifier	%	Classification (GHS-US)
ISOOCTANE UNLABELED	(CAS No)540-84-1	99.9986	Flam. Liq. 1, H224 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

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	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
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	: Rinse skin with water/shower. Remove/Take off immediately all contaminated clothing. Wash with plenty of soap and water. Wash contaminated clothing before reuse. If skin irritation occurs: Wash with plenty of soap and water. Get medical advice/attention. Specific treatment (see Hazard pictograms (CLP) on this label).
First-aid measures after eye contact	: Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.
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

# 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

ECN-5267

## 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

### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

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

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

Fire hazard : Extremely flammable liquid and vapor.  
Explosion hazard : May form flammable/explosive vapor-air mixture.

#### 5.3. Advice for firefighters

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

No additional information available

##### 6.1.2. For emergency responders

Protective equipment : Avoid breathing dust, mist or spray.

#### 6.2. Environmental precautions

Avoid release to the environment.

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

No additional information available

#### 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. Avoid breathing dust, mist or spray.  
Hygiene measures : Wash Both hands thoroughly after handling.

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

Technical measures : 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

No additional information available

#### 8.2. Exposure controls

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



Hand protection : Wear suitable protective clothing and 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.

# 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

ECN-5267

## 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

### 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	: 114.23
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	: -107 °C (- 161 °F)
Freezing point	: No data available
Boiling point	: 99 °C (210 °F)
Flash point	: -12 °C (10 °F) - closed cup
Self ignition temperature	: 396 °C (745 °F)
Decomposition temperature	: No data available
Flammability (solid, gas)	: Extremely flammable liquid and vapor
Vapor pressure	: 55 hPa (41 mmHg) at 21 °C (70 °F)
Relative vapor density at 20 °C	: 3.94 - (Air = 1.0)
Relative density	: No data available
Solubility	: Water: 0 %
Log Pow	: No data available
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	: 1 - 6 % (V)

#### 9.2. Other information

No additional information available

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

No additional information available

#### 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

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

#### 10.5. Incompatible materials

No additional information available

#### 10.6. Hazardous decomposition products

May release flammable gases.

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

Acute toxicity : Not classified

#### 1,2,3,4,5,8-HEXACN (13C10, 99%) (103426-93-3 (Unlabeled))

ATE (oral)	500.000 mg/kg body weight
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Skin corrosion/irritation : Causes skin irritation.

Serious eye damage/irritation : Not classified

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ECN-5267

## 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

Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
Specific target organ toxicity (single exposure)	: May cause drowsiness or dizziness.
Specific target organ toxicity (repeated exposure)	: Not classified
Aspiration hazard	: May be fatal if swallowed and enters airways.
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

Ecology - water : Very toxic to aquatic life with long lasting effects.

### 12.2. Persistence and degradability

#### 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

Persistence and degradability	May cause long-term adverse effects in the environment.
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#### 1,2,3,4,5,8-HEXACN (13C10, 99%) (103426-93-3 (Unlabeled))

Persistence and degradability	Not available.
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#### ISOOCTANE UNLABELED (540-84-1)

Persistence and degradability	Not available.
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### 12.3. Bioaccumulative potential

#### 1,2,3,4,5,8-HEXACN (13C10, 99%) (103426-93-3 (Unlabeled))

Bioaccumulative potential	Not available.
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#### ISOOCTANE UNLABELED (540-84-1)

Bioaccumulative potential	Not available.
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### 12.4. Mobility in soil

#### 1,2,3,4,5,8-HEXACN (13C10, 99%) (103426-93-3 (Unlabeled))

Ecology - soil	Not available.
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#### ISOOCTANE UNLABELED (540-84-1)

Ecology - soil	Not available.
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### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Other adverse effects

No additional information available

## 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)	: 1262
DOT NA no.	UN1262

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## ECN-5267

### 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

#### 14.2. UN proper shipping name

DOT Proper Shipping Name : Octanes  
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) : II - Medium Danger  
DOT Special Provisions (49 CFR 172.102) : IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). 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.  
T4 - 2.65 178.274(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) : 202  
DOT Packaging Bulk (49 CFR 173.xxx) : 242

#### 14.3. Additional information

Other information : No supplementary information available.

#### Overland transport

Packing group (ADR) : II  
Class (ADR) : 3 - Flammable liquid  
Hazard identification number (Kemler No.) : 33  
Classification code (ADR) : F1  
Danger labels (ADR) : 3 - Flammable liquids



Orange plates : An orange rectangular label with a black border. It is divided into two horizontal sections. The top section contains the number '33' in black, and the bottom section contains the number '1262' in black.

Tunnel restriction code : D/E  
Limited quantities (ADR) : 1L  
EAC : 3YE  
Excepted quantities (ADR) : E2

#### Transport by sea

DOT Vessel Stowage Location : B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.  
MFAG-No : 128

#### Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 5 L  
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 L  
Civil Aeronautics Law : Flammable liquids

# 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

ECN-5267

## 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

### 14.4. Environmental hazards

Dangerous for the environment :



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

#### 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard Delayed (chronic) health hazard
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#### ISOOCTANE UNLABELED (540-84-1)

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

#### CANADA

#### 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE

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

#### 15.2.1. National regulations

No additional information available

### 15.3. US State regulations

#### 1,2,3,4,5,8-HEXACN (PCN-65) (13C10, 99%) 10 UG/ML IN ISOOCTANE()

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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#### ISOOCTANE UNLABELED (540-84-1)

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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## 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.



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## ECN-5267

### 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

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

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
Aquatic Chronic 2	Hazardous to the aquatic environment - Chronic Hazard Category 2
Asp. Tox. 1	Aspiration hazard Category 1
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Flam. Liq. 1	Flammable liquids Category 1
Flam. Liq. 2	Flammable liquids Category 2
Skin Irrit. 2	skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H224	Extremely flammable liquid and vapor
H225	Highly 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
H335	May cause respiratory irritation
H336	May cause drowsiness or dizziness
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects
H411	Toxic to aquatic life with long lasting effects
R11	Highly flammable
R22	Harmful if swallowed
R36/37	Irritating to eyes and respiratory system
R38	Irritating to skin
R41	Risk of serious damage to eyes
R50/53	Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment
R51/53	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment
R67	Vapors may cause drowsiness and dizziness
F	Highly flammable
N	Dangerous for the environment
Xi	Irritant
Xn	Harmful

NFPA health hazard

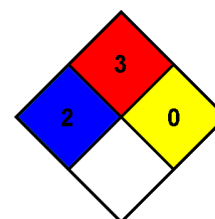
: 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.

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*