

#### SAFETY DATA SHEET

# SECTION 1 - IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

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Canada)

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accepted)

Product identifier Hemisqualane

**Synonyms**  $C_{13-15}$  alkane; hydrogenated farnesene; farnesane;

2,6,10-trimethyldodecane; dodecane, 2,6,10-trimethyl; TMD

**Trade name** Neossance<sup>TM</sup> Hemisqualane HF

Chemical family Branched paraffinic hydrocarbons

**REACH Registration No.:** 01-2119948111-47-0000; 01-2119948111-47-0001

Relevant identified uses of the substance or mixture and uses

advised against

Used as an emollient and/or solvent in cosmetics. Not for human or animal

consumption.

**Issue Date** 20 July 2015

## **SECTION 2 - HAZARDS IDENTIFICATION**

**GHS** Classification of the substance or mixture

**Regulation** (EC) 1272/2008 Aspiration hazard - Category 1. Substance not yet fully tested. OSHA HCS 2012

#### Label elements

CLP/GHS hazard pictogram



**CLP/GHS signal word** Danger

**CLP/GHS** hazard statements

H304 - May be fatal if swallowed and enters airways.

**CLP/GHS** precautionary

statements

P102: Keep out of reach of children. P301+P310 - If swallowed: Immediately contact a poison control center or physician. P331- Do NOT induce vomiting. P405 - Store locked up. P501 - Dispose of contents/container to location in

accordance with local/regional/ national/international regulations.

**NFPA Classification:** Health Hazard: 1; Fire Hazard: 1; Reactivity Hazard; 0

Other hazards See Section 11.

Note The toxicological properties of this substance have not been fully characterized.

#### **SECTION 3 - COMPOSITION/INFORMATION ON INGREDIENTS**

<u>Ingredient</u>	CAS#	EINECS/	<b>Amount</b>	<u>EU</u>	GHS /CLP
		ELINCS#		Classification	Classification
Hemisqualane	3891-98-3	622-542-2	>95%	R65	AH1: H304

See Section 16 for full text of GHS/CLP classifications. The EU classification is Note

> based on Directive 67/548/EEC and the GHS classification is based on Regulation (EC) 1272/2008 (EU CLP) and 29 OSHA 1910.1200 (United Nations ST/SG/AC 10/30 rev 3). See Section 15 for additional

clarification on CAS and regulatory status.

# **SECTION 4 - FIRST AID MEASURES**

Description of first aid measures

**Immediate Medical** 

**Attention Needed** 

Yes

**Eye Contact** If easy to do, remove contact lenses, if worn. Immediately flush eyes with

copious quantities of water for at least 15 minutes. If irritation occurs or persists,

notify medical personnel and supervisor.

Skin Contact Wash exposed area with soap and water and remove contaminated

clothing/shoes. If irritation occurs or persists, notify medical personnel and

supervisor.

Inhalation Immediately move exposed subject to fresh air. If not breathing, give artificial

respiration. If breathing is labored, administer oxygen. Immediately notify

medical personnel and supervisor.

If swallowed, call a physician immediately. Do not induce vomiting unless **Ingestion** 

> directed by medical personnel. Do not give anything to drink unless directed by medical personnel. Never give anything by mouth to an unconscious person.

Notify medical personnel and supervisor.

Protection of first aid

responders

See Section 8 for Exposure Controls/Personal Protection recommendations.

Most important symptoms and effects, both acute and delayed

See Sections 2 and 11

**Indication of immediate** medical attention and necessary

Treat symptomatically and supportively. If accidental exposure occurs to an individual who is also taking one or more concomitant medications, consult the **special treatment needed, if** respective package or prescribing information for potential drug interactions.

**SECTION 5 - FIREFIGHTING MEASURES** 

**Extinguishing media** Use water spray (fog), foam, dry powder, or carbon dioxide, as appropriate for

surrounding fire and materials.

Specific hazards arising from the substance or

mixture

No information identified. May emit toxic fumes of carbon monoxide and carbon

dioxide.

Flammability/Explosivity No explosivity or flammability data identified. High airborne concentrations of

finely divided organic particles can potentially explode if ignited.

Advice for firefighters Wear full protective clothing and a self-contained breathing apparatus with a full

facepiece operated in the pressure demand or other positive pressure mode.

Decontaminate all equipment after use.

#### SECTION 6 - ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures If product is released or spilled, take proper precautions to minimize exposure by using appropriate personal protective equipment (see Section 8). Area should be adequately ventilated.

**Environmental precautions** Do not empty into drains. Avoid release to the environment. Contact the National

Response Center in case of accidental discharge to waterways that produce a

sheen.

Methods and material for containment and cleaning up

For small spills (such as in a laboratory), soak up material with absorbent, e.g., damp paper towel, and wash spill area thoroughly with soap and water. For large spills in manufacturing, absorb liquid with an appropriate adsorbent. Do not raise dust. Eliminate ignition sources. Use only equipment suitable for use with combustible liquids. Place spill materials into a leak-proof container suitable for disposal. Dispose of material in a manner that is compliant with federal, state and local laws.

**Reference to other sections** See Sections 8 and 13 for more information.

## **SECTION 7 - HANDLING AND STORAGE**

**Precautions for safe handling** Avoid contact with eyes, skin and other mucous membranes. Wash thoroughly

after handling. Use personal protective equipment. Avoid breathing vapor. Do not eat, drink or smoke while handling this product. Avoid prolonged or repeated exposure. Provide sufficient air exchange and/or exhaust in workrooms. Take precautionary measures against static discharges and use proper bonding and grounding procedures. Use normal preventative fire protection measures. Do not

cut or weld empty containers as they may contain a residue.

**Conditions for safe storage** 

including any incompatibilities

Keep container tightly closed. Keep in a cool and well ventilated area away from any ignition source. To maintain product quality, do not store in heat or direct

sunlight.

**Specific end use(s)** As a solvent or emollient for cosmetics.

#### SECTION 8 - EXPOSURE CONTROLS/PERSONAL PROTECTION

**Control Parameters** 

**Occupational Exposure Limits** 

<u>Compound</u> <u>Issuer</u> <u>Type</u> <u>OEL</u> Hemisqualane -- -- --

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**DNEL/PNEC Limits** A DNEL/PNEC is not required. The main potential hazard from hemisqualane is from

accidental ingestion and a DNEL is not required. No hazards have been identified for

the environment (see Section 12).

**Risk Management Measures** Do not ingest. If swallowed then seek immediate medical assistance. Keep away from

children.

**Exposure/Engineering controls** Provide ventilation. Use local exhaust and/or enclosure at mist/

aerosol/spray-generating points. High-energy operations such as spraying should be

done within an approved emission control or containment system.

**Respiratory protection** If adequate ventilation is unavailable, use a NIOSH approved N95 or P95 dust mask or

an approved and properly fitted air-purifying respirator with organic vapor cartridge based on an assessment of risk and exposure level. Choice of respiratory protection should be appropriate to the task and the level of existing engineering controls.

**Hand protection** Wear nitrile or other impervious gloves if skin contact is possible.

**Skin protection** Wear appropriate gloves, lab coat, or other protective overgarment if skin contact is

likely. Base the choice of skin protection on the job activity, potential for skin contact

and solvents and reagents in use.

**Eye/face protection** Wear safety glasses with side shields, chemical splash goggles, or full face shield, if

necessary. Base the choice of protection on the job activity and potential for contact

with eyes or face. An emergency eye wash station should be available.

**Environmental Exposure** 

**Controls** 

Avoid release to the environment and operate within closed systems wherever practicable. Air and liquid emissions should be directed to appropriate pollution control devices. In case of spill, do not release to drains. Implement appropriate and effective emergency response procedures to prevent release and inadvertent contact

by personnel.

Other protective measures Wash hands in the event of contact with this substance, especially before eating,

drinking or smoking. Protective equipment is not to be worn outside the work area (e.g., in common areas or out-of-doors). Decontaminate all protective equipment

following use.

#### **SECTION 9 - PHYSICAL AND CHEMICAL PROPERTIES**

# Information on basic physical and chemical properties

**Appearance** Liquid

**Color** Colorless

**Odor** Nearly odorless

**Odor threshold** No information identified.

**pH** No information identified.

Melting point/freezing point No information identified.

Initial boiling point and

boiling range

241-251°C at 760 mm Hg (ASTM D86)

**Flash point** 110 °C (230 °F) (ASTM D93)

**Evaporation rate** No information identified.

**Flammability** (solid, gas) No information identified.

Upper/lower flammability or LFL @ 25°C 0.48 (ASTM E681)

explosive limits UFL @25°C 7.0 (ASTM E681)

Vapor pressure 89.3 Pa at 20°C (ASTM 2879)

Vapor density No information identified.

**Relative density** 0.77 g/cm3 at 15 °C. (ASTM D4052)

Water solubility 0.25 μg/L (literature reference).

**Solvent solubility** Soluble in alcohols.

 $Partition\ coefficient\ (log)$ 

(n-octanol/water)

7.49 at 25 °C (estimated)

**Auto-ignition temperature** 197 °C (387 °F) (ASTM E659)

**Decomposition temperature** No information identified.

Viscosity (kinematic) 2.325 mm2/s @ 40 °C (ASTM D445)

**Explosive properties** No information identified.

Oxidizing properties No information identified.

Other information

Molecular weight 212.41

**Molecular formula**  $C_{15}H_{32}$ 

#### **SECTION 10 - STABILITY AND REACTIVITY**

**Reactivity** No information identified.

**Chemical stability** Stable under normal handling and storage conditions.

Possibility of hazardous

reactions

Not expected to occur.

**Conditions to avoid** Keep away from heat, sparks, and open flame.

**Incompatible materials** Strong oxidizers.

Hazardous decomposition

products

No information identified.

#### **SECTION 11 - TOXICOLOGICAL INFORMATION**

# Information on toxicological

effects

**Route of entry** May be absorbed by inhalation, skin contact and ingestion.

**Acute toxicity** 

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**Irritation/Corrosion** Hemisqualane may cause dermal irritation. In *in vitro* eye and skin tests (MatTek

Epiocular<sup>TM</sup> MTT viability assay, MatTek Epiderm<sup>TM</sup> skin irritation test) hemisqualane was non-irritating. In human 48 hour patch testing, hemisqualane was considered non irritating. In HRIPT, irritation was noted as the pure substance under highly localized and occluded conditions. At lower concentrations or with

open application, mild to no irritation was observed; no irritation was observed at

concentrations of up to 60%.

**Sensitization** In three human repeated patch studies, hemisqualane was not considered to be a

sensitizer ranging from concentrations of 20% to 80%. Hemisqualane was not

sensitizing by the Local Lymph Node Assay (40% max concentration).

**STOT-single exposure** No studies identified.

STOT-repeated

exposure/Repeat-dose

toxicity

No studies identified.

**Reproductive toxicity** No studies identified. **Developmental toxicity** No studies identified.

**Genotoxicity** Negative in an Ames bacterial cell mutagenicity assay and mouse lymphoma

assay. Not clastogenic at non-precipitating doses with or without metabolic

activation in the chromosome aberration study.

**Carcinogenicity** No studies identified. This substance is not listed by NTP, IARC, ACGIH or

OSHA as a carcinogen.

**Aspiration hazard** Considered to be an aspiration hazard based on kinematic viscosity.

**Human health data** See Irritation and Sensitization sections.

**Additional information** Substance not yet fully tested.

#### **SECTION 12 - ECOLOGICAL INFORMATION**

**Aquatic Toxicity** Hemisqualane is not classified for acute or chronic toxicity to aquatic species.

Hemisqualane is essentially insoluble in water (0.25  $\mu$ g/L) and is not expected to hydrolyse. It was tested in chronic fish and daphnia studies and no toxicity occurred

at the limit of water solubility (0.25  $\mu$ g/L).

Additional toxicity information Based on the results from similar substances, hemisqualane is not expected to

inhibit the activity of sewage sludge micro-organisms.

Persistence and Degradability In CO<sub>2</sub>-evolution ready biodegradability tests (OECD301B), hemisqualane

degradation was between 12-44% by 28 days. In addition, modelled data

(EpiSiuite v 4.11, BIOWIN v4.10 and BioHCWin v1.01), predict that hemisqualane will not be readily biodegradable, that it will be ultimately biodegradable in a period of weeks to months and that its half-life is 22 days. The measured half-life in

a seawater biodegradation study was 3.5 days (CONCAWE).

**Bioaccumulative potential** Predicted range 1074 to 1944 L/kg wet-wt by modelling (EpiSuite v4.11 and

BCFBAF v3.01). Based on predicted values of less than 2000 L/kg wet-wt

hemisqualane is not expected to bioaccumulate.

Mobility in soil Not expected to be mobile in soil. Predicted log Koc: 6.5 (Kowwin method)

Results of PBT and vPvB

assessment

Based on the chemical safety assessment and the results described herein,

hemisqualane is not a PBT / vPvB substance.

Other adverse effects No data available.

**Note** The environmental characteristics of this substance have not been fully

investigated. Releases to the environment should be avoided.

## **SECTION 13 - DISPOSAL CONSIDERATIONS**

Waste treatment methods Used product should be disposed of according to local, state, and federal

regulations. Do not send down the drain or flush down the toilet. All wastes containing the material should be properly labeled. Dispose of wastes in accordance to prescribed federal, state, and local guidelines, e.g., appropriately permitted chemical waste incinerator. Rinse waters resulting from spill cleanups should be discharged in an environmentally safe manner, e.g., appropriately permitted municipal or on-site wastewater treatment facility.

**SECTION 14 - TRANSPORT INFORMATION** 

**Transport** Based on the available data, this substance is not regulated as a hazardous material/

dangerous good under EU ADR/RID, US DOT, Canada TDG, IATA, or IMDG.

**UN number** None assigned.

**UN proper shipping name** None assigned.

Transport hazard classes and

packing group

None assigned.

**Environmental hazards** Based on the available data, this substance is not regulated as an environmental

hazard or a marine pollutant.

**Special precautions for users** Substance not fully tested - avoid exposure and releases to the environment.

Transport in bulk according to Annex II of MARPOL73/78 and

the IBC Code

Not applicable.

#### **SECTION 15 - REGULATORY INFORMATION**

Safety, health and environmental regulations/legislation specific for the substance or mixture This SDS complies with the requirements under US, EU and GHS (EU CLP - Regulation EC No 1272/2008) guidelines. Consult your local or regional

authorities for more information.

Chemical safety assessment Conducted.

**OSHA Hazardous** Harmful or fatal if swallowed. Can enter lungs and cause damage.

WHMIS classification This substance does not meet any of the hazard criteria of the Controlled Products

Regulations and the SDS contains all of the information required by those

regulations.

**US FFDCA**  $C_{13-15}$  alkane.

**US TSCA status** Listed on the TSCA inventory as Dodecane, 2,6,10-trimethyl-

**EU REACH** REACH registration number: 01-2119948111-47-0000; 01-2119948111-47-0001

**China 2014 IECIC**  $C_{13-15}$  alkane.

SARA section 313 Not listed.

California proposition 65 Not listed.

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#### **SECTION 16 - OTHER INFORMATION**

Full text of H phrases, P phrases and GHS classification

AH1- Aspiration Hazard - Category 1 H304 - May be fatal if swallowed and enters airways.

Sources of data

Information from published literature and internal company data.

**Abbreviations** 

ACGIH - American Conference of Governmental Industrial Hygienists ADR/RID - European Agreement Concerning the International Carriage of Dangerous Goods by Road/Rail AIHA - American Industrial Hygiene Association CAS# - Chemical Abstract Services Number CLP - Classification, Labelling, and Packaging of Substances and Mixtures DNEL - Derived No Effect Level DOT - Department of Transportation EINECS - European Inventory of New and Existing Chemical Substances ELINCS - European List of Notified Chemical Substances

EU - European Union GHS - Globally Harmonized System of Classification and Labelling of Chemicals HRIPT – Human Repeated Insult Patch Test IARC - International Agency for Research on Cancer IDLH - Immediately Dangerous to Life or Health IATA - International Air Transport Association IMDG - International Maritime Dangerous Goods LOEL - Lowest Observed Effect Level LOAEL - Lowest Observed Adverse Effect Level NIOSH - The National Institute for Occupational Safety and Health NOEL - No Observed Effect Level NOAEL - No Observed Adverse Effect Level NTP - National Toxicology Program OEL - Occupational Exposure Limit OSHA - Occupational Safety and Health Administration PBT - Persistent, Bioaccumulative and Toxic PNEC - Predicted No Effect Concentration SARA - Superfund Amendments and Reauthorization Act STEL - Short Term Exposure Limit TDG - Transport Dangerous Goods TSCA - Toxic Substances Control Act TWA - Time Weighted Average WHMIS - Workplace Hazardous Materials Information System

Revisions

This is the fifth version of this SDS.

Disclaimer

The above information is based on data available to us and is believed to be correct. Since the information may be applied under conditions beyond our control and with which we may be unfamiliar, we do not assume any responsibility for the results of its use and all persons receiving it must make their own determination of the effects, properties and protections which pertain to their particular conditions. No representation, warranty, or guarantee, express or implied (including a warranty of fitness or merchantability for a particular purpose), is made with respect to the materials, the accuracy of this information, the results to be obtained from the use thereof, or the hazards connected with the use of the material. Caution should be used in the handling and use of the material because it is a chemical substance. The above information is offered in good faith and with the belief that it is accurate. As of the date of issuance, we are providing all information relevant to the foreseeable handling of the material. However, in the event of an adverse incident associated with this product, this Safety Data Sheet is not, and is not intended to be, a substitute for consultation with appropriately trained personnel.