SAFETY DATA SHEET

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

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Product identifier Hemisqualane

Synonyms C_{13}-C_{15} alkane; 2,6,10-trimethyldodecane; dodecane, 2,6,10-trimethyl ; farnesane; TMD

Trade names Neossance™ Hemisqualane

Chemical family Branched paraffinic hydrocarbons

REACH Registration No.: 01-2119948111-47-0000 (new submission number PE483357-29)

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.

Note The pharmacologic and toxicologic properties of this substance have not been fully characterized; this SDS will be revisited as more data become available.

Issue Date 10 April 2014

SECTION 2 - HAZARDS IDENTIFICATION

GHS Classification of the substance or mixture

Regulation (EC) 1272/2008 [GHS] Aspiration hazard - Category 1. Substance not yet fully tested.

Label elements

CLP/GHS hazard pictogram

CLP/GHS signal word Danger

CLP/GHS hazard statements H304 - May be fatal if swallowed and enters airways.

SECTION 2 - HAZARDS IDENTIFICATION …continued

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	This substance should be considered hazardous according to Regulation (EC) No 1272/2008 (EU CLP) and United Nations ST/SG/AC 10/30 rev 3 applicable GHS regulations. The pharmacologic and toxicologic properties of this substance have not been fully characterized. See Section 16 for full text of GHS classifications.

SECTION 3 - COMPOSITION/INFORMATION ON INGREDIENTS

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

Note See Section 16 for full text of GHS/CLP classifications. The GHS/CLP classification is based on Regulation (EC) 1272/2008 and 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.
Ingestion	If swallowed, call a physician immediately. Do not induce vomiting unless 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.

SECTION 4 - FIRST AID MEASURES

Most important symptoms and effects, both acute and delayed	See Sections 2 and 11
Indication of immediate medical attention and special treatment needed, if necessary	Treat symptomatically and supportively. If accidental exposure occurs to an individual who is also taking one or more concomitant medications, consult the 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.
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, use an industrial vacuum cleaner equipped with a high efficiency particulate (HEPA) filter if available. Alternatively if in solid or dried form, do not raise dust. Surround spill or powder with absorbents and place a damp cloth or towel over the area to minimize powder from entering the air. Add excess liquid to allow for the material to enter solution. Capture remaining liquid onto spill absorbents. Place spill materials into a leak-proof container suitable for disposal. Decontaminate area a second time. 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. Use normal preventative fire protection measures.

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) No information identified.

SECTION 8 - EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Occupational Exposure Limits

Compound	Issuer	Type	OEL
Hemisqualane	--	--	--

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

Exposure/Engineering controls Selection and use of containment devices and personal protective equipment should be based on a risk assessment of exposure potential. 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 Choice of respiratory protection should be appropriate to the task and the level of existing engineering controls. An approved and properly fitted air-purifying respirator with HEPA filters should provide ancillary protection based on the known or foreseeable limitations of existing engineering controls. Use a powered air-purifying respirator equipped with HEPA filters or combination filters or a positive-pressure air-supplied respirator if there is any potential for an uncontrolled release, when exposure levels are not known, or in any other circumstances where a lower level of respiratory protection may not provide adequate protection.

Hand protection Wear nitrile or other impervious gloves if skin contact is possible. When the material is dissolved or suspended in an organic solvent, wear gloves that provide protection against the solvent.

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 or spread of contamination and to prevent inadvertent contact by personnel.

SECTION 8 - EXPOSURE CONTROLS/PERSONAL PROTECTION

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	Paraffinic
Odor threshold	No information identified.
pH	No information identified.
Melting point/freezing point	No information identified.
Initial boiling point and boiling range	198°C at 760 mm Hg
Flash point	110 °C (230 °F)
Evaporation rate	No information identified.
Flammability (solid, gas)	No information identified.
Upper/lower flammability or explosive limits	LFL @ 25°C 0.48 UFL @25°C 7.0
Vapor pressure	89.3 Pa at 20°C
Vapor density	No information identified.
Relative density	0.77 g/cm3 at 15 °C.
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)
Decomposition temperature	No information identified.
Viscosity (kinematic)	2.325 mm2/s @ 40 °C
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

Compound	Type	Route	Species	Dose
Hemisqualane	LC_{50}	Inhalation	Rat	>2.19 mg/L
	LD_{50}	Oral	Rat	> 5000 mg/kg
	LD_{50}	Dermal	Rabbit	> 5000 mg/kg

Irritation/Corrosion In rabbits, hemisqualane was not considered an irritant under GHS or CLP. In *in vitro* eye and skin tests (MatTek Epiocular™ MTT viability assay, MatTek Epiderm™ 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%.

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. 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

Toxicity Hemisqualane is not classified for acute or chronic toxicity to aquatic species. Hemisqualane is essentially insoluble in water (0.25 µg/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 µg/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_2-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.

SECTION 14 - TRANSPORT INFORMATION …continued

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.
Chemical safety assessment	Conducted.
OSHA Hazardous	Harmful or fatal if swallowed. Can enter lungs and cause damage. Substance not fully tested.
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}-C_{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 (new submission number PE483357-29)
China 2014 IECIC	C_{13}-C_{15} alkane.
SARA section 313	Not listed.
California proposition 65	Not listed.

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

SECTION 16 - OTHER INFORMATION …continued

Abbreviations …continued

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 first 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.